Comparative Methods of Computing Maximum Likelihood Estimates for Non-Linear Econometric Systems

by

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To

My Mother

and the Fond Memory of

My Dear Father

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ABSTRACT

This research is mainly concerned with numerical optimisation techniques applied to general non-linear econometric simultaneous equations systems. The method of estimation used is maximum likelihood. An estimation program which applies gradient-type procedures, specifically the Berndt-Hall-Hall-Hausman and Gill-Murray-Pitfield methods, is developed. This program allows the estimation of a general small-to-medium size model which is non-linear in parameters, variables or both. In the course of program development, a general differentiation program is written which will differentiate a set of econometric equations and thus provide the analytical gradients for the optimisation procedures. A comparative study has been made of the relative efficiency of the two methods by running a set of simulated non-linear models and also using a small macro-economic model of the British Economy specified by David F. Hendry. To improve the efficiency of the estimation program in terms of computing time, the Berndt-Hall-Hall-Hausman method was implemented on the ICL Distributed Array Processor (DAP) which employs parallel computations. The DAP runs show that for a model with a large sample size, the DAP is approximately 30 times faster than the conventional computer CDC 7600, but that for the present algorithm, the latter is a more efficient alternative for small sample sizes.

CONTENTS

Acknowledgements 3

Abstract 4

Chapter 1 Survey and Literature 9

1.0 Introduction 9

1.1 Maximum Likelihood Estimator for Non-Linear Econometric Systems 10

1.2 Numerical Optimisation Applied to Non-Linear Econometric Models 16

1.3 Specific Application Program 18

Chapter 2 Numerical Optimisation Techniques For Non-Linear Econometric Models 21

2.0 Numerical Optimisation 21

2.1 Optimisation Methods 21

2.2 Minimisation With Derivatives 23

2.2.1 The Newton-Raphson Method 24

2.2.2 Variable-metric Methods 33

2.2.3 General Gradient Method 35

2.2.4 The Method of Fletcher and Powell (DFP) .. 36

2.2.5 The Complementary DFP Updating Formula (CompDFP) 38

2.2.6 Gill-Murray-Pitfield Method (GMP) 39

2.2.7 The BHHH Hessian Approximation 42

2.3 Minimisation Without Derivatives 44

2.3.1 Conjugate Direction Methods 44

2.3.2 Variable-metric Methods 47

2.3.3 Comments Regarding Minimisation Without Derivatives 51

2.4 Choice of Line Search 52

2.4.1 Quadratic Interpolation 53

2.4.2 Cubic Interpolation 57

2.4.3 Bard Line Search 58

2.4.4 The BHHH Line Search 60

2.4.5 Efficiency and Termination 61

2.5 Choice of Stopping Criterion 62

2.5.1 The Gradient Stopping Criterion 62

2.5.2 The Weighted-Gradient Stopping Criterion . 64

Chapter 3 Characteristics of Econometric Estimation Problems 66

3.0 The Model 66

3.1 The BHHH Method of Estimation and Inference by Maximum Likelihood 70

3.2 The BHHH Algorithm 74

Chapter 4 A Method of Specification, Differentiation and Computation for Sets of General Functions 77

4.0 A Differentiation Program 77

4.1 Organisation of the Differentiation Program 77

4.2 General Considerations and Function Specifications 78

4.3 Sets of Conventions for Defining A Function 82

4.4 Differentiation 95

4.5 Simplification 98

4.6 Numerical Evaluation of Function and Derivative Values 98

4.7 Example 99

Chapter 5 A Computer Program For The Estimation of General Non-Linear Econometric Models 103

5.0 An Estimation Program 103

5.1 Organisation of the Estimation Program 104

5.2 Functional Definitions 106

5.3 Estimation Methods 107

5.4 Program Composition 108

Chapter 6 Non-Linear Econometric Modelling on a Parallel Processor 112

6.1 Potential Role of the Distributed Array Processor for Research in Economics 112

6.2 The Distributed Array Processor (DAP) 115

6.3 Architecture 115

6.4 Programming the DAP 116

6.5 Examples 118

6.6 Estimation Procedure and Implementation (Timings and Results in Section 7.7) 121

Chapter 7 A Set of Non-Linear Models 125

7.0 Non-Linear Models Simulations 125

7.1 Modelling Considerations 126

7.2 Model Specification 127

7.3 Data Generation Process 130

7.4 Sets of Models 132

7.5 Alternative Values of Parameters 135

7.6 Estimation Results and Computer Timings 137

7.7 Results and Timings for Models (iii) on the Distributed Array Processor 163

Chapter 8 An Aggregate Demand Model for the United Kingdom, 1957-1967 167

8.0 A Demand Model 167

8.1 The Model (Linear Form) 167

8.2 Transformation of Model (Non-Linear Form) 169

8.3 Treatment of Coefficients for Equation u_1 and Constants for all equations 171

8.4 Deseasonised Data Series 174

8.5 NLMLE Specification of Model 176

8.6 Results 177

Chapter 9 General Conclusion 182

Appendix A Cholesky Factorisation 186

Appendix B NLMLE Listing 193

Appendix C A User's Guide to NLMLE 244

Appendix D Program Output - A Typical Run From Model (iii) . 246

Appendix E A Parallel Inversion Routine 252

Appendix F Sets of Non-Linear Models 256

References 259

CHAPTER 1

SURVEY AND LITERATURE

1. Introduction

This research is concerned with the estimation of general non-linear simultaneous equations econometric models by the method of maximum likelihood.

A computer program called Non-Linear Maximum Likelihood Estimation (NLMLE) is specifically developed for this purpose. This program allows the estimation of a quite general non-linear model by the method of Berndt-Hall-Hall-Hausman (BHHH, 1974) or alternatively by the use of the Gill-Murray-Pitfield (GMP, 1972) algorithm (with or without derivatives) from the NAG library. In the course of program development, a differentiation program is developed which will differentiate a set of functions defined by general FORTRAN specifications to any order (Sargan and Chong (1980)). After developing the main estimation program, where much effort has been concentrated on finding an efficient line search algorithm by the use of quadratic interpolation (Powell, 1964), comparison has been made of the relative efficiency of the two methods (BHHH and GMP) by applying these to simulated data from a representative set of models. A more realistic model (Hendry, 1974) has also been studied. At this stage is appeared clear that the BHHH method provides generally a better optimisation algorithm when the number of parameters in the model is greater than 8 and the sample size is greater than 50.

The program is written in FORTRAN IV and the serial version has been implemented on CDC 7600 and ICL 2980 computer systems. For DAP

(Distributed Array Processor) application using parallel processing, a few subroutines from the existing program have been reorganised and reprogrammed in DAPFORTRAN. Due to the storage restrictions of the DAP (2 Mbyte), the program is restricted to the estimation models with no more than 5 equations and 30 parameters but up to 4096 observations. It became clear that the use of DAP will be advantageous when the sample size is large, ideally close to 4096 observations. To increase the degree of parallelism and extend the program size will require further research which is beyond the scope of the present studies.

As the program (the serial version) is written in FORTRAN IV, it is fairly portable; one would expect without much difficulty to implement it on other computer systems.

In the following sections, we will briefly review the literature on maximum likelihood estimators, on numerical methods applied to non-linear econometric models and, lastly, formula manipulation and symbolic differentiation on a computer.

1.1 Maximum Likelihood Estimator for Non-linear Econometric Systems

The usual method of formulating a model which is generally non-linear in both the variables and the parameters in a form suitable for maximum likelihood estimation is that suggested initially by Eisenpress and Greenstadt (1966). For a later discussion, see Chow (1973). The full-information maximum likelihood estimates of the k-vector of unknown parameters θ can be obtained as the parameter $\hat{\theta}$ that maximises the concentrated log-likelihood function of simultaneous equations systems that are non-linear in the parameters and/or variables.

Each equation of the simultaneous equation system is specified by expressing the error on the equation as a general function of the variables and the parameters, and it is then assumed that the errors are jointly normally distributed.

The Eisenpress and Greenstadt procedure is to estimate each equation in a non-linear system by ordinary least squares, and then to use these results as the initial approximation to a full-information solution. However, the problem of identification in non-linear systems is not treated and provision has to be made ultimately to avoid working with under-identified equations and systems. In Eisenpress and Greenstadt's work, they define a given equation in the form

$$\begin{aligned} y_{it} = g_i(&y_{1t}, \ldots, y_{i-1,t}, y_{i+1,t}, \ldots, y_{Nt}, \\ &z_{1t}, \ldots, z_{Mt}, \theta_1, \ldots, \theta_K) + u_{it} \end{aligned} \qquad (1.1)$$

where one endogenous variable y_i is an arbitrary function g_i of the other endogenous variables, the predetermined variables z_m and the parameters θ_k subject to a random disturbance u_i. Then least squares or maximum likelihood estimation (if the u_i are assumed normal) is applied to the T observations on the y's and z's, to estimate the θ's, under the assumption that

$$E(u_{it}) = 0, \qquad t = 1, \ldots, T$$

$$Cov(u_{it}u_{it'}) = \begin{cases} 0 & t \neq t' \\ \sigma^2_{u_i} & t = t' \end{cases}$$

The estimates of the θ's will, in general, be inconsistent, but this calculation is able to provide a first guess for use in the techniques that follow.

To obtain the least-squares estimates of the θ's, the function

$$L' = \sum_t (y_{it} - g_i)^2$$

is minimised with respect to the θ's, using the modified Newton method which requires the first and second derivatives of L' with respect to θ.

On more general assumptions, the full-information maximum likelihood estimates are obtained by defining the set of equations as

$$f_{it}(y_t, z_t, \theta) \equiv f_{it}(y_{1t}, \dots, y_{Nt}, z_{1t}, \dots, z_{Mt}; \theta_1, \dots, \theta_K) = u_{it} \qquad (1.2)$$

$$i = 1, \dots, N; \; t = 1, \dots, T$$

where u_{it} are the random disturbances of these relations. The f's are assumed to have derivatives up to third order.

The concentrated log-likelihood function of (1.2) is

$$L^*(\theta) = \text{const} - \frac{T}{2} \log\det(S) + \sum_t \log |\det(J_t)| \qquad (1.3)$$

where

f_t is the $N \times 1$ vector with elements f_{it},

$S \equiv S(\theta) = (\frac{1}{T} \sum_t f_{it}(\theta) f_{jt}(\theta))$, and J_t is the $N \times N$ Jacobian matrix,

$$J_t \equiv J_t(\theta) = \left(\frac{\partial f_t(y_t, z_t, \theta)}{\partial y_t} \right) .$$

To maximise $L^*(\theta)$, the gradient method or modified Newton method is used. These both make use of the first and second derivatives of $L^*(\theta)$ with respect to the θ's. As in many iterative procedures, the first approximation and the conditioning of various matrices (e.g. the Hessian) are important in determining the speed of convergence. Usually any arbitrary first guess for θ will be accepted by the algorithms, but a good first guess may speed up convergence substantially.

Chow (1973) generalises the modified Newton method for the computation of full-information maximum likelihood estimates of parameters of a system of linear structural equations to the case of a system of non-linear structural equations. The main differences of Chow's approach to that of Eisenpress and Greenstadt are:

(1) Eisenpress' and Greenstadt's basic formulation is more general, assuming that all parameters in the system may appear in every equation (see equation 1.2), whereas Chow assumes as the basic set-up that there is a distinct set of parameters belonging to each equation. His basic formulation is as follows:
Let the g^{th} function

$$f_{gt}(y_{1t},\ldots,y_{Nt}; \beta_g)$$

of the G dependent variables and $K = N - G$ predetermined variables $y_{1t},\ldots,y_{Nt}$ at period t and of the row vector β_g of N_g unknown parameters to be equated to a residual u_{gt} $(g = 1,\ldots,G)$.

Assume u_{gt} is normally distributed with means zero and covariances $E(u_{gt}u_{hs}) = \delta_{ts}\sigma_{gh}$. For T observations, the concentrated log-likelihood function L is proportional to

$$-\frac{T}{2}\log|S| + \sum_{t=1}^{T}\log|B_t^o| ,$$

where

$$S \equiv (S_{gh}) = (\frac{1}{T}\sum_t u_{gt}u_{ht})$$

and

$$B_t^o \equiv (\beta_{gh,t}^o) = \left(\frac{\partial u_{gt}}{\partial y_{ht}}\right)$$

(2) Partly because of his formulation, Chow obtains simpler and more explicit expressions for the derivatives of the likelihood functions.

(3) Again, partly because of his formulation, the problem of linear restriction on the parameters in the same equation or in different equations can be conveniently dealt with by Chow.

(4) Chow's paper features the treatments of identities in the system and of residuals which may follow an autoregressive scheme.

An extensive derivation of the estimation equations for non-linear systems is given under the assumptions that each structural equation contains a distinct set of parameters, that the parameters are not subject to any linear restrictions, and that the (additive) residuals are serially uncorrelated. It also provides the treatment of the special case when some equations are linear, and contrasts this case with the non-linear case.

Berndt-Hall-Hall-Hausman (1974) propose an ingenious idea of using the statistical relation that the covariance matrix of the maximum likelihood estimator is equal to the inverse of the covariance matrix of the gradient of the log-likelihood function, which in its turn is equal to minus the (inverse) Hessian matrix of the log-likelihood function. Their algorithm requires much less computation than previous algorithms and unlike previous algorithms is less likely to fail from instability of the iterative procedure. We will concentrate our studies on the BHHH method and will derive the estimation equations in Chapter 3.

Amemiya (1977) proves the consistency and the asymptotic normality of the maximum likelihood estimator in the general non-linear simultaneous equation model. The proof depends on the assumption that the errors are normally distributed which is not necessary for simultaneous equation models which are linear in the variables. It is also proved that the maximum liklihood estimator is asymptotically more efficient than the non-linear three stage least squares estimator providing the specification is correct. However, the latter has the advantage of being consistent even when the normality assumption is removed.

Hatanaka (1978) proposes a full-information estimation method for macro-economic models which are generally non-linear in variables. The method is shown to be asymptotically efficient and feasible in terms of computer computations, and hopefully it may be applied to the undersized sample case. The idea of the BHHH method may be applied to replace the Hessian of the two-step scoring estimator which is asymptotically equivalent to the maximum likelihood estimator.

1.2 Numerical Optimisation Applied to Non-linear Econometric Models

Bard (1970) investigates several of the best known gradient methods, and the performance of these methods is compared in the solution of some least squares maximum likelihood, and Bayesian estimation problems. He concludes that modifications of the Gauss method (including Marquardt's) performed best, followed by variable metric rank one and Davidon-Fletcher-Powell methods, in that order. There appeared to be no need to locate the optimum precisely in the one-dimensional searches, but the matrix inversion method used with the Gauss algorithm must guarantee a positive definite inverse.

Sargan and Sylwestrowicz (1976) develop a specialised numerical optimisation computer program for the estimation of simultaneous equation econometric models, in the hope that it would be more efficient than the alternative computing methods. The methods are compared by estimating a small macro-economic model of the British economy as specified by Hendry (1974) with five different sets of assumptions as to the stochastic processes generating the errors of the equations. All the assumptions involve separate single equation autoregressive equations, explaining the current error on each equation in terms of the previous error on the same equation. This was chosen as giving experience of the use of the optimisation program on a representative problem, from the point of view of time and complication in computing the required function, and with a number of parameters to be estimated which is reasonably large as most econometric models involve a large number of parameters.

To maximise the likelihood function appropriate to a simultaneous linear equations model, a subroutine is provided to calculate the likelihood function and use this with a general optimisation routine not requiring analytical derivatives, such as the Powell conjugate directions method. It is also possible to use the Davidon-Fletcher-Powell type of quasi-Newton method, providing it with a subroutine to calculate the likelihood function and its first derivatives; and finally a special generalised Gauss-Newton program was written for use with the non-linear simultaneous equation likelihood functions.

The extensive results presented in the paper indicate that the Gill-Murray-Pitfield optimisation routine, making use of analytic first derivatives, is the most efficient method with most of the models.

Belsley (1980) examines some important elements in calculating the non-linear full-information maximum likelihood estimator which produce substantial reductions in computational cost. The choice of optimiser, method of Hessian approximation, choice of convergence criterion and exploitation of sparsity of matrices are all investigated.

It is concluded that the Newton-Raphson algorithm employing an analytical computed Hessian is computationally much more efficient than Davidon-Fletcher-Powell. The weighted gradient stopping criterion is recommended, that is,

$$-g'H^{-1}g \leq \varepsilon$$

where

g is the gradient of the likelihood of function $L(\underline{\theta})$,

H is the Hessian matrix of $L(\underline{\theta})$,

ε is the tolerance level of accuracy.

Exploiting the sparsity of J_t (the Jacobian) and the efficient calculation of the components that make up the analytic Hessian are also investigated for large models.

1.3 Specific Application Program

In order to implement a general optimisation procedure of the BHHH kind on the computer, we need to be able to specify the general functions

$$f_{it}\,(y_t, z_t, \theta) = u_{it}$$

in a suitable computer code form so that we can differentiate these functions twice analytically w.r.t. θ, that is, $\partial f_i(y_t, z_t, \theta)/\partial\theta$ and $\partial^2 f_i(y_t, z_t, \theta)/\partial\theta\partial\theta'$.

It is of considerable importance that the resulting form of function specification should lead to efficient evaluation of both functions and their derivatives. It is not necessary that the derivatives should be presented in the most logical form from the point of view of mathematical interpretation, but unnecessary repetitive computing should be avoided in the course of their evaluation.

Obviously it would be a bad strategy to differentiate the set of functions explicitly and then input the derivatives to the computer for evaluation for the following reasons:

1. The functions can be very complex.

2. There exists a high probability of differentiation and programming errors.

3. For each model, we need to differentiate and program the functions and derivatives. The volume of arithmetic involved could be very intense, for example, it takes several function evaluations in the line search just to reduce the function value.

Therefore an automatic differentiation program is necessary to compute the set of econometric functions and their derivatives. Most programs for automatic differentiation are embedded in general computer packages for symbol manipulation, for example, systems such as MACSYMA and REDUCE (see references). These are used for performing symbolic as well as numerical mathematical manipulations. With such computer packages, it is possible to differentiate, integrate, take limits, solve systems of linear or polynomial equations, factor polynomials, expand functions in Taylor series, solve differential equations and perform many other operations.

Since it is intended that the differentiations of the set of econometric functions is to be carried out on the computer in order that complicated functions are differentiated accurately with results which are easy to understand and compute numerically, and to avoid unnecessary repetitive computation in the process, systems as comprehensive as MACSYMA and REDUCE would not be appropriate for this application. Moreover, it is necessary to have a compact set of derivatives of the concentrated log-likelihood function for our estimation procedures, it would be difficult to extract the necessary subrountines from these packages in order to perform the same task.

However, we are very much influenced by the function specifications and data structures of these systems, and have decided to develop our own differentiation program (see Chapter 4) with the specific application of differentiating and evaluating non-linear econometric functions.

This program is written in FORTRAN IV and is machine portable. It permits natural mathematical notation in FORTRAN definitions and can differentiate a set of functions with respect to a given set of variables up to any order. Only numerical values of the functions and derivatives are printed instead of the symbolic form of the expression in mathematical notation. It is hoped that it could be easily implemented with any non-linear econometric estimation programs written in FORTRAN IV. The program was specifically written so that it could be developed on the CDC 7600 computer, and then transferred with minimal rewriting onto the ICL 2980 system with the Distributed Array Processor (DAP).

CHAPTER 2

NUMERICAL OPTIMISATION TECHNIQUES FOR NON-LINEAR ECONOMETRIC MODELS

2. Numerical Optimisation

Many issues arise in the practical task of optimising a non-linear function. A general description of these may be found in Goldfeld and Quandt (1972), Jacoby et al. (1972), Murray (1972), and Bard (1970). In this chapter, we examine two issues that are among the more important and interesting in the optimisation of the concentrated log-likelihood function, relevant to the non-linear full-information maximum likelihood (NLFIML) estimator, namely, the choice of the optimisation method and the method of approximating the Hessian.

2.1 Optimisation Methods

Two different optimisation algorithms are compared in separate runs for the various models. The gradient-type method (e.g. BHHH) and the quasi-Newton method (e.g. GMP). Each of these algorithms is a Newton-like procedure in that its step in the parameter space at each iteration could be a Newton-like step,

$$d\underline{\theta}^{(k)} \equiv \underline{\theta}^{(k+1)} - \underline{\theta}^{(k)} = -\lambda^{(k)}\left[\underline{H}^{(k)}(\underline{\theta})\right]^{-1}\underline{g}^{(k)}(\underline{\theta}) \qquad (2.1)$$

where

$\lambda^{(k)}$ = a scalar, the step-length along the search direction

$H^{(k)}(\underline{\theta})$ a $K \times K$ matrix; the Hessian $\left.\frac{\partial^2 L^*(\underline{\theta})}{\partial \underline{\theta} \partial \underline{\theta}'}\right|_{\underline{\theta}=\underline{\theta}^{(k)}}$

or approximate Hessian at the k^{th} iteration.

$\underline{g}^{(k)}(\underline{\theta})$ = a K-vector; the gradient of $L^*(\underline{\theta})$ evaluated at the k^{th} iteration, $\left.\frac{\partial L^*(\underline{\theta})}{\partial \underline{\theta}}\right|_{\underline{\theta}=\underline{\theta}^{(k)}}$

There are, of course, many ingenious non-Newton optimisation techniques that require no first or second derivatives. Such algorithms have been developed to handle general optimisation problems. However, when a specific functional form for the objective function is known, as is the case here in the concentrated log-likelihood function, it is generally concluded that it is beneficial to exploit this information. Thus, we examine closely methods that use at least gradient information. We also examine methods that use numerical approximation to the gradient to see how relatively inefficient they may be.

The Hessian H of (2.1) plays two important roles in maximum-likelihood estimation, and the means for its calculation or approximation can affect both. First, the Hessian is used numerically. Either the Hessian or its approximation is used at each iteration of a Newton-like optimisation algorithm to determine the next step in (2.1). Second, the Hessian is used statistically. At the maximum-likelihood solution, the negative of the inverse Hessian provides an estimate of the asymptotic variance-covariance matrix of $\underline{\theta}$.

2.2 Minimisation with Derivatives

We use the notation $\phi(\underline{\theta}) = -L^*(\underline{\theta})$ defined as the concentrated log-likelihood function whose least value is to be calculated, where $\underline{\theta}$ is a vector whose components are the variables which are to be adjusted automatically by a minimisation algorithm. Let n be the number of components of $\underline{\theta}$. To define $\phi(\underline{\theta})$ for a minimisation algorithm, the user must provide a subroutine that calculates $\phi(\underline{\theta})$ for any $\underline{\theta}$. He must also provide a starting vector $\underline{\theta}^{(o)}$, say, and perhaps some other information, for example, step-lengths and the accuracy required. Then most algorithms automatically construct a sequence of points $\underline{\theta}^{(k)}$ $(k = 1, 2, \ldots)$, which should converge to the required vector of variables.

The algorimthms that we consider are iterative, and we let $\underline{\theta}^{(k)}$ be the starting point of the k^th^ iteration. They include safeguards which force the inequality

$$\phi(\underline{\theta}^{(k+1)}) \leq \phi(\underline{\theta}^{(k)}) \qquad (2.2)$$

to be satisfied.

We assume that the function $\phi(\underline{\theta})$ has continuous first and second derivatives. In this case it is almost always best to select the minimisation algorithm from the general methods that are designed to work particularly well when $\phi(\underline{\theta})$ is a quadratic function. The reason is that if the steps $\{\underline{\theta}^{(k+1)} - \underline{\theta}^{(k)}\}$ become small, then usually the local behaviour of $\phi(\underline{\theta})$ is similar to that of a quadratic function, so the algorithm should work well, and if the steps $\{\underline{\theta}^{(k+1)} - \underline{\theta}^{(k)}\}$ are large then usually good progress is being made anyway.

Some very useful algorithms of this type are described in the books by Brent (1973) and Kowalik and Osborne (1968).

2.2.1 The Newton-Raphson Method

When $G^{(k)}(\underline{\theta}) = [H^{(k)}(\underline{\theta})]^{-1}$, where $H^{(k)}$ is the exact Hessian matrix at $\underline{\theta}^{(k)}$, we have the Newton-Raphson method which is described in the following algorithm.

(a) Algorithm 2.1

It is assumed that an initial estimate $\underline{\theta}^{(o)}$ of the optimum point $\underline{\theta}^*$ is known.

Step 0: Set $k = 0$

Step 1: Compute $\underline{g}^{(k)}(\underline{\theta})$, and $H^{(k)}(\underline{\theta})$ from

$$\underline{g}^{(k)}(\underline{\theta}) = \left.\frac{\partial\phi(\underline{\theta})}{\partial\underline{\theta}}\right|_{\underline{\theta}=\underline{\theta}^{(k)}}$$

$$H^{(k)}(\underline{\theta}) = \left.\frac{\partial^2\phi(\underline{\theta})}{\partial\underline{\theta}\partial\underline{\theta}'}\right|_{\underline{\theta}=\underline{\theta}^{(k)}}$$

Step 2: Compute $\underline{p}^{(k)}$ by solving the system of linear equations

$$H^{(k)}(\underline{\theta})\underline{p}^{(k)} = -\underline{g}^{(k)}(\underline{\theta})$$

Step 3: Compute $\underline{\theta}^{(k+1)}$ from

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} + \underline{p}^{(k)}$$

Step 4: If convergence has been attained, stop, else set $k = k+1$ and go to Step 1.

(b) Safeguarding the Method of Newton-Raphson

The sequence $\{\underline{\theta}^{(k)}\}$ generated from Algorithm 2.1 will converge to a critical point $\underline{\theta}^*$ of ϕ which is a strong local minimiser of ϕ if $\underline{\theta}^{(o)}$ is sufficiently close to $\underline{\theta}^*$, and the order of convergence is quadratic. Unfortunately, however, a sufficiently good initial estimate $\underline{\theta}^{(o)}$ of $\underline{\theta}^*$ is often not available. In order to make Newton's method more satisfactory for practical use, devices must be incorporated into Algorithm 2.1 which reduce the probability of divergence. We shall consider the principal causes of failure in Newton's method.

We have the descent direction $\underline{p}^{(k)}$ defined by

$$\underline{p}^{(k)} = -[H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta}) \tag{2.3}$$

where $H^{(k)}(\underline{\theta})$ and $\underline{g}^{(k)}(\underline{\theta})$ are the Hessian matrix and gradient vector respectively for the function ϕ at $\underline{\theta}^{(k)}$,

If $[H^{(k)}(\underline{\theta})]^{-1}$ exists, then $G^{(k)}(\underline{\theta}) = [H^{(k)}(\underline{\theta})]^{-1}$ is positive definite if and only if $H^{(k)}(\underline{\theta})$ is positive definite. If $G^{(k)}(\underline{\theta})$ is positive definite then

$$\underline{g}^{(k)\prime}(\underline{\theta})\underline{p}^{(k)} = -\underline{g}^{(k)\prime}(\underline{\theta})[G^{(k)}(\underline{\theta})]\underline{g}^{(k)}(\underline{\theta}) < 0$$

so that $p^{(k)}$ is downhill for ϕ at $\underline{\theta}^{(k)}$. If, however, ϕ is not well approximated by a quadratic function, in the neighbourhood of $\underline{\theta}^{(k)}$, then the step $\underline{p}^{(k)}$ to $\underline{\theta}^{(k+1)}$ may be too large, in that $\phi(\underline{\theta}^{(k+1)}) > \phi(\underline{\theta}^{(k)})$ and the minimisation has not progressed smoothly.

If $[H^{(k)}(\underline{\theta})]^{-1}$ exists but is not positive definite it may be that although the Newton step $\underline{p}^{(k)}$ is well defined, we have $\underline{g}^{(k)'}(\underline{\theta})\underline{p}^{(k)} = 0$. In this case although $\underline{p}^{(k)}$ is not actually uphill for ϕ at $\underline{\theta}^{(k)}$ we cannot be sure that $\phi(\underline{\theta}^{(k+1)}) < \phi(\underline{\theta}^{(k)})$.

If $\underline{g}^{(k)'}(\underline{\theta})\underline{p}^{(k)} > 0$, then $\underline{p}^{(k)}$ is uphill for ϕ at $\underline{\theta}^{(k)}$, and no step in the direction $\underline{p}^{(k)}$ can help the minimisation.

If $[H^{(k)}(\underline{\theta})]^{-1}$ does not exist then $\underline{p}^{(k)}$ is not even defined, so that if further progress is to be made we need an alternative method for constructing $\underline{p}^{(k)}$ when $G^{(k)}(\underline{\theta})$ is singular.

It is clear that the Newton sequence $\{\underline{\theta}^{(k)}\}$, if it converges at all, it converges to a critical point of ϕ. But the sequence $\{\underline{\theta}^{(k)}\}$ may converge to a saddle point or to a maximiser of ϕ instead of a minimiser, although this does not usually happen if $\underline{\theta}^{(o)}$ is sufficiently close to a minimiser of ϕ.

We may conclude from the above discussion that Newton's method is subject to the following causes of failure during the $(k + 1)$th iteration.

1. $G^{(k)}(\underline{\theta})$ exists and is positive definite but $\underline{p}^{(k)}$ is too large and $\phi(\underline{\theta}^{(k+1)}) > \phi(\underline{\theta}^{(k)})$.

2. The direction $\underline{p}^{(k)}$ is orthogonal to $\underline{g}^{(k)}(\underline{\theta})$.

3. $G^{(k)}(\underline{\theta})$ exists but is not positive definite.

4. $G^{(k)}(\underline{\theta})$ does not exist.

To reduce the probability of failure due to the causes above, we consider the following strategies.

1. If $[G^{(k)}(\underline{\theta})]$ is positive definite then $\underline{p}^{(k)}$ is downhill for ϕ at $\underline{\theta}^{(k)}$ and there exists $\lambda > 0$ sufficiently small such that

$$\phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)}) < \phi(\underline{\theta}^{(k)}). \qquad (2.4)$$

If the length of $\underline{p}^{(k)}$ is so small that ϕ is well approximated by a quadratic function throughout the range of $\underline{\theta}^{(k)}$ to $\underline{\theta}^{(k+1)}$ then it is likely that

$$\phi(\underline{\theta}^{(k)} + \underline{p}^{(k)}) < \phi(\underline{\theta}^{(k)}).$$

If, however,

$$\phi(\underline{\theta}^{(k)} + \underline{p}^{(k)}) > \phi(\underline{\theta}^{(k)})$$

then a value of $\lambda^{(k)} \in (0,1)$ must be found such that

$$\phi(\underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}) < \phi(\underline{\theta}^{(k)}) \qquad (2.5)$$

A simple strategy for computing a value of $\lambda^{(k)}$ which satisfies (2.5) is given in the following algorithm.

Notice that if $\lambda^{(k)}$ is becoming very small and (2.5) is not satisfied, the algorithm then terminates.

<u>Algorithm 2.2</u>

```
1.  Set $\lambda = 1$.

2.  Compute $\phi$ from $\phi = \phi(\underline{\theta}^{(k)} + \lambda \underline{p}^{(k)})$.

3.  If $\phi < \phi(\underline{\theta}^{(k)})$ go to 6.

4.  If $\lambda \leq 10^{-5}$ go to 7.

5.  Set $\lambda = \frac{\lambda}{2}$ and go to 2.

6.  Set $\lambda^{(k)} = \lambda$, and $\phi(\underline{\theta}^{(k+1)}) = \phi$.

    Return to Newton-Raphson routine.

7.  Stop.
```

An alternative, and perhaps more natural strategy is to compute $\lambda^{(k)}$ by performing a line search along $\underline{p}^{(k)}$ if $\underline{p}^{(k)}$ is known to be downhill for ϕ at $\underline{\theta}^{(k)}$. The introduction of the parameter $\lambda^{(k)}$ computed according to Algorithm 2.2 or by performing a line search (see section 2.4) safeguards Newton's method against cause 1 of failure.

2. Consider now if $\underline{p}^{(k)}$ is orthogonal to $\underline{g}^{(k)}(\underline{\theta})$ and no progress can be made by performing a line search along $\underline{p}^{(k)}$. This illustrates cause 2 of failure. In practice, owing to rounding error, effective orthogonality of $\underline{p}^{(k)}$ and $\underline{g}^{(k)}(\underline{\theta})$ is decided by determining whether $|\underline{g}^{(k)'}(\underline{\theta})\underline{p}^{(k)}| \leq \varepsilon \, ||\underline{g}^{(k)}(\underline{\theta})||_2 ||\underline{p}^{(k)}||_2$, where $\varepsilon > 0$ is a given small number relative to unity. One strategy for safeguarding Newton's method against cause 2 of failure is to replace $\underline{p}^{(k)}$ with $-\underline{g}^{(k)}(\underline{\theta})$ if $|\underline{g}^{(k)'}(\underline{\theta})\underline{p}^{(k)}| \leq \varepsilon \, ||\underline{g}^{(k)}(\underline{\theta})||_2 ||\underline{p}^{(k)}||_2$ and perform a line search

along the new $\underline{p}^{(k)}$. Thus if $\underline{g}^{(k)}(\underline{\theta})$ and $[G^{(k)}(\underline{\theta})]\underline{g}^{(k)}(\underline{\theta})$ are effectively orthogonal, we take a steepest descent step.

3. If $G^{(k)}(\underline{\theta})$ is not positive definite, then $\underline{p}^{(k)}$ is not necessarily downhill and the existence of $\lambda^{(k)} > 0$ which satisfies (2.5) cannot be guaranteed.

If $\underline{g}^{(k)'}\underline{p}^{(k)} > 0$, then $\underline{p}^{(k)}$ is uphill at $\underline{\theta}^{(k)}$ and $-\underline{p}^{(k)}$ therefore downhill. In this case we replace $\underline{p}^{(k)}$ defined by (2.3) with $-\underline{p}^{(k)}$ and the existence of $\lambda > 0$ such that $\phi(\lambda) < \phi(0)$ is guaranteed. It is a better strategy to replace $\underline{p}^{(k)}$ with $-\underline{p}^{(k)}$ if $\underline{g}^{(k)'}\underline{p}^{(k)} > 0$ than rejecting $\underline{p}^{(k)}$ altogether and taking a steepest descent step. This strategy therefore safeguards Newton's method against cause 3 of failure.

4. If $H^{(k)}(\underline{\theta})$ is singular, then $\underline{p}^{(k)}$ given by (2.4) is not defined. A simple strategy for overcoming this difficulty is to replace $\underline{p}^{(k)}$ with $-\underline{g}^{(k)}(\underline{\theta})$ and take a steepest descent step,

thus safeguarding Newton's method against cause 4 of failure.

From the preceding discussion, we obtain the following algorithm.

Algorithm 2.3

It is assumed that an estimate $\underline{\theta}^{(o)}$ of a minimiser $\underline{\theta}^*$ of ϕ and $\varepsilon > 0$ are given.

Step 0: Set $k = 0$.

Step 1: Compute $\underline{g}^{(k)}(\underline{\theta})$, and $H^{(k)}(\underline{\theta})$ from

$$\underline{g}^{(k)}(\underline{\theta}) = \left. \frac{\partial\phi(\underline{\theta})}{\partial\underline{\theta}} \right|_{\underline{\theta}=\underline{\theta}^{(k)}}$$

$$H^{(k)}(\underline{\theta}) = \left. \frac{\partial^2\phi(\underline{\theta})}{\partial\underline{\theta}\partial\underline{\theta}'} \right|_{\underline{\theta}=\underline{\theta}^{(k)}}$$

Step 2: If $H^{(k)}(\underline{\theta})$ is singular, go to Step 10.

Step 3: Compute $\underline{p}^{(k)}$ from

$$\underline{p}^{(k)} = - [H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta})$$

Step 4: If $|\underline{g}^{(k)'}(\underline{\theta})\,\underline{p}^{(k)}| \leq \varepsilon\, \|\underline{g}^{(k)}(\underline{\theta})\|_2 \|\underline{p}^{(k)}\|_2$, then go to Step 10.

Step 5: If $\underline{g}^{(k)'}(\underline{\theta})\,\underline{p}^{(k)} > \varepsilon\, \|\underline{g}^{(k)}(\underline{\theta})\|_2 \|\underline{p}^{(k)}\|_2$, then go to Step 12.

Step 6: Compute $\lambda^{(k)}$ by repeated bisection (Algorithm 2.2) or by performing a line search (section 2.4).

Step 7: Set $\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}$.

Step 8: If convergence is attained, go to Step 13.

Step 9: Set $k = k + 1$, go to Step 1.

Step 10: Set $\underline{p}^{(k)} = -\underline{g}^{(k)}(\underline{\theta})$.

Step 11: Perform a line search along $\underline{p}^{(k)}$ to obtain $\lambda^{(k)}$, and go to Step 7.

Step 12: Set $\underline{p}^{(k)} = -\underline{p}^{(k)}$ and go to Step 6.

Step 13: Set $\underline{\theta}^* = \underline{\theta}^{(k+1)}$.

Step 14: Stop.

(c) <u>Objections to Newton-Raphson Method</u>

There are a number of objections to Newton's method as a computational procedure, the most important of which are as follows.

1. In order to evaluate $H^{(k)}(\underline{\theta})$, we must compute $n(n+1)/2$ function values $\left.\frac{\partial^2\phi(\underline{\theta})}{\partial\underline{\theta}\partial\underline{\theta}'}\right|_{\underline{\theta}=\underline{\theta}^{(k)}}$. This means that $n(n+1)/2$ partial derivatives must be calculated analytically and programmed, with consequent probability of analytical and programming error. Also storage space must be allocated in

the computer for $n(n+1)/2$ numbers, and for a subprogram which is required in order to compute them. And the time required for these calculations may be very large (especially when estimating econometric models).

2. At each iteration, $[H^{(k)}(\underline{\theta})]^{-1}$ must be computed. This requires $O(n^3)$ arithmetic operations. Also a subprogram for inverting matrices is required.

3. It may be that $H^{(k)}(\underline{\theta})$ is singular for some k so that the method breaks down.

4. The method is not guaranteed to converge unless $\underline{\theta}^{(o)}$ is sufficiently close to $\underline{\theta}^*$.

Note : We have in fact safeguarded objections 3 and 4.

These objections frequently make Newton's method unsuitable for numerical calculation, but if a sufficiently good initial estimate $\underline{\theta}^{(o)}$ of $\underline{\theta}^*$ is known, and if the first and second partial derivatives of ϕ are easy to program and to compute, then the method is among the best which is available. On the other hand, if $\underline{\theta}^{(o)}$ is far from $\underline{\theta}^*$, then there is no reason to believe that in the first few iterations the method has any advantages over a comparatively crude algorithm which takes much less time than the Newton-Raphson.

Objection 1 may to some extent be overcome by using a numerical differentiation formula in order to estimate the Hessian matrix, but n additional evaluations of $\underline{g}^{(k)}(\underline{\theta})$ are required for the computation of $H^{(k)}(\underline{\theta})$. The use of a numerical differentiation formula may be inefficient if n is large or if the computational labour required for the evaluation of $\underline{g}^{(k)}(\underline{\theta})$ is large and also $\underline{g}^{(k)}(\underline{\theta})$ could be inaccurate.

The preceding considerations provide a motive for constructing methods for minimising ϕ in which it is not necessary to compute or invert $H^{(k)}(\underline{\theta})$, but which have superlinear[1] convergence, since they ultimately find a value of $H^{(k)}(\underline{\theta})$ which approximates the exact Hessian when $\underline{\theta}$ is close to $\underline{\theta}^*$.

2.2.2 Variable-Metric Methods

In these methods, the matrix $[H^{(k)}(\underline{\theta})]^{-1}$ is replaced by a positive definite symmetric matrix $G^{(k)}(\underline{\theta})$ calculated from currently available quantities such as $\underline{\theta}^{(k)}$, $\underline{g}^{(k)}(\underline{\theta})$, $\underline{\theta}^{(k-1)}$, and $\underline{g}^{(k-1)}(\underline{\theta})$, to compute $\underline{\theta}^{(k+1)}$ from

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} - \lambda^{(k)} G^{(k)}(\underline{\theta})\underline{g}^{(k)}(\underline{\theta}) \qquad (2.6)$$

If $G^{(k)}(\theta)$ is positive definite $(\forall k \geq 0)$, then $-G^{(k)}(\underline{\theta})\underline{g}^{(k)}(\underline{\theta})$ is downhill for ϕ at $\underline{\theta}^{(k)}$, because $-\underline{g}^{(k)'}(\underline{\theta})G^{(k)}(\underline{\theta})\underline{g}^{(k)}(\underline{\theta}) < 0$ if $\underline{g}^{(k)}(\underline{\theta}) \neq 0$. Therefore if $G^{(k)}(\underline{\theta})$ is positive definite and $\underline{g}^{(k)}(\underline{\theta}) \neq 0$, there exists $\lambda^{(k)} > 0$ such that

$$\phi(\underline{\theta}^{(k)} - \lambda^{(k)} G^{(k)}(\underline{\theta})\underline{g}^{(k)}(\underline{\theta})) < \phi(\underline{\theta}^{(k)})$$

A method for overcoming to some extent objection 4 to Newton's method therefore consists of generating $\{\underline{\theta}^{(k)}\}$ from (2.6).

The use of (2.6) also overcomes objection 3 to Newton's method because even though the Hessian is singular, $G^{(k+1)}(\underline{\theta})$ can be defined so that it not only exists but is positive definite.

The following algorithm is a general **variable metric method for** minimising ϕ.

---

[1] It may be possible to make statements about the rate of convergence that occurs. Let $\underline{\theta}^*$ to be the local minimum point. Define the error

$$e^{(k)} = \underline{\theta}^{(k)} - \underline{\theta}^*.$$

If $e^{(k)} \to 0$, that means convergence. For instance, if $||e^{(k+1)}||/||e^{(k)}|| \to a$, then the rate of convergence is said to be <u>linear</u> or <u>first order</u> if $a \geqslant 0$, and <u>Superlinear</u> if $a = 0$. Clearly it is desirable to have a as small as possible. In some cases it is possible to show that $||e^{(k+1)}||/||e^{(k)}||^2 \to a$ in which case the rate is said to be <u>quadratic</u> or <u>second order</u>. This is even more rapid since the error decreases as the square of the previous error.

Algorithm 2.4

It is assumed that $\underline{\theta}^{(o)}$ and $G^{(o)}$ are given.

Step 0: Set $k = 0$.

Step 1: Compute $\phi^{(k)}(\underline{\theta})$ and $\underline{g}^{(k)}(\underline{\theta})$ from

$$\phi^{(k)}(\underline{\theta}) = \phi(\underline{\theta}^{(k)})$$

$$\underline{g}^{(k)}(\underline{\theta}) = \underline{g}(\underline{\theta}^{(k)})$$

Step 2: Compute $\underline{p}^{(k)} = - G^{(k)}(\underline{\theta})\underline{g}^{(k)}(\underline{\theta})$.

Step 3: Compute $\lambda^{(k)}$ such that

$$\phi(\underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}) = \min_{\lambda} \phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)})$$

Step 4: Compute $\underline{\theta}^{(k+1)}$ from

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}$$

Step 5: Compute $\underline{g}^{(k+1)}(\underline{\theta})$, $\underline{s}^{(k)}$ and $y^{(k)}$ from

$$\underline{g}^{(k+1)}(\underline{\theta}) = \underline{g}(\underline{\theta}^{(k+1)})$$

$$\underline{s}^{(k)} = \underline{\theta}^{(k+1)} - \underline{\theta}^{(k)}$$

and

$$y^{(k)} = \underline{g}^{(k+1)}(\underline{\theta}) - \underline{g}^{(k)}(\underline{\theta})$$

Step 6: Compute $G^{(k+1)}(\underline{\theta})$ from

$$G^{(k+1)}(\underline{\theta}) = G^{(k)}(\underline{\theta}) + \Pi_1 z^{(k)} z^{(k)'} + \Pi_2 \omega^{(k)} \omega^{(k)'}$$

where $z^{(k)}$, $\omega^{(k)}$ are $n \times 1$ vectors and Π_1, Π_2 are scalars. The exact values of these variables, which are functions of $\underline{g}^{(k)}(\underline{\theta})$, $\underline{p}^{(k)}$ and $\underline{g}^{(k+1)}(\underline{\theta})$, will depend upon the modification rule used.

Therefore Algorithm 2.4 contains a class of methods rather than a single variable-metric method. Many updating formulae of the type in Step 6 have been proposed since Davidon (1959) described the first variable-metric method. In this chapter some of the most successful variable-metric methods will be described.

2.2.3 General Gradient Method

At the beginning of the k^{th} iteration, we possess a current value of $\underline{\theta}^{(k)}$ and we seek a new $\underline{\theta}^{(k+1)}$ using the formula

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} - \lambda^{(k)} G^{(k)}(\underline{\theta}) \underline{g}^{(k)}(\theta) \qquad (2.7)$$

where

$\underline{g}^{(k)}(\underline{\theta})$ is the gradient vector of $\phi(\underline{\theta})$ at $\underline{\theta} = \underline{\theta}^{(k)}$

$\lambda^{(k)}$ is a scalar that minimises $\phi(\underline{\theta}^{(k)} - \lambda G^{(k)}(\theta)\underline{g}^{(k)}(\underline{\theta}))$,

and $G^{(k)}(\underline{\theta})$ is a positive definite matrix which guarantees that if $\underline{g}^{(k)}(\underline{\theta}) \neq 0$, then for sufficiently small positive $\lambda^{(k)}$, we have satisfied the condition (2.2).

$G^{(k)}(\underline{\theta})$ should be some approximation to $[H^{(k)}(\underline{\theta})]^{-1}$, where $H^{(k)}(\underline{\theta})$ is the Hessian matrix of ϕ at $\underline{\theta} = \underline{\theta}^{(k)}$.

2.2.4 The Method of Fletcher and Powell (DFP)

The method of Fletcher and Powell (1963) is an improved version of a method due to Davidon (1959). It is still one of the best methods for unconstrained minimisation in which only the gradient vector of the objective function is required.

The matrix $G^{(k+1)}(\underline{\theta})$ is given by the updating formula

$$G^{(k+1)}(\underline{\theta}) = G^{(k)}(\underline{\theta}) + \frac{\lambda^{(k)}\underline{p}^{(k)}\underline{p}^{(k)'}}{\underline{p}^{(k)'}\underline{y}^{(k)}} - \frac{G^{(k)}(\underline{\theta})\underline{y}^{(k)}\underline{y}^{(k)'}G^{(k)}(\underline{\theta})}{\underline{y}^{(k)'}G^{(k)}(\underline{\theta})\underline{y}^{(k)}} \qquad (2.8)$$

We now show that (2.8) does correspond to the general algorithm as defined above.

If Householder's (1964) rank-one modification rule is applied first to

$$\bar{G}^{(k)}(\underline{\theta}) = G^{(k)}(\underline{\theta}) + \frac{\lambda^{(k)}\underline{p}^{(k)}\underline{p}^{(k)'}}{\underline{p}^{(k)'}\underline{y}^{(k)}}$$

and then to

$$G^{(k+1)}(\underline{\theta}) = \bar{G}^{(k)}(\underline{\theta}) - \frac{G^{(k)}(\underline{\theta})\underline{y}^{(k)}\underline{y}^{(k)'}G^{(k)}(\underline{\theta})}{\underline{y}^{(k)'}G^{(k)}(\underline{\theta})\underline{y}^{(k)}},$$

the corresponding recurrence relation for the approximate Hessian matrix is obtained

$$H^{(k+1)}(\underline{\theta}) = H^{(k)}(\underline{\theta}) + \left(\frac{1}{\delta\lambda} - \frac{\eta}{\delta^2}\right)\underline{y}^{(k)}\underline{y}^{(k)'} +$$

$$\frac{1}{\delta}\left\{\underline{g}^{(k)}(\underline{\theta})\underline{y}^{(k)'} + \underline{y}^{(k)}\underline{g}^{(k)'}(\underline{\theta})\right\} \qquad (2.9)$$

where

$$\eta = \underline{g}^{(k)'}(\underline{\theta})\underline{p}^{(k)}$$

and

$$\delta = \underline{y}^{(k)'}\underline{p}^{(k)}$$

If an exact line search is made then $\underline{g}^{(k+1)'}(\underline{\theta})\underline{p}^{(k)} = 0$, but since this cannot be guaranteed in practice, δ is taken as

$$\delta = \underline{g}^{(k+1)'}(\underline{\theta})\underline{p}^{(k)} - \eta$$

To show how equation (2.9) can be written as a particular form of the equation defined in Step 6, define

$$t = \mu\underline{g}^{(k)}(\underline{\theta}) + \frac{1}{\mu\delta}\underline{y}^{(k)}$$

where μ is an undetermined constant. Then

$$tt' = \frac{1}{\delta}\left(\underline{g}^{(k)}(\underline{\theta})\underline{y}^{(k)'} + \underline{y}^{(k)}\underline{g}^{(k)'}(\underline{\theta})\right) + \mu^2\underline{g}^{(k)}(\underline{\theta})\underline{g}^{(k)'}(\underline{\theta}) + \frac{1}{\mu^2\delta^2}\underline{y}^{(k)}\underline{y}^{(k)'}$$

This formula can be used with (2.9) to give

$$H^{(k+1)}(\underline{\theta}) = H^{(k)}(\underline{\theta}) + \left(\frac{1}{\delta\lambda} - \frac{\eta}{\delta^2} - \frac{1}{\mu^2\delta^2}\right)\underline{y}^{(k)}\underline{y}^{(k)'} + tt' - \mu^2\underline{g}^{(k)}(\underline{\theta})\underline{g}^{(k)'}(\underline{\theta})$$

Now the coefficient of $\underline{y}^{(k)}\underline{y}^{(k)'}$ can be made equal to zero by choosing μ to satisfy

$$\mu^2 = \frac{\lambda}{\delta - \lambda\eta}$$

or

$$\mu^2 = \frac{\lambda}{\underline{g}^{(k+1)'}(\underline{\theta})\underline{p}^{(k)} - (\lambda + 1)\underline{g}^{(k)'}(\underline{\theta})\underline{p}^{(k)}}$$

Thus we get the recurrence relation

$$H^{(k+1)} = H^{(k)} + \frac{1}{\mu^2\delta^2}\bar{t}\bar{t}' - \mu^2\underline{g}^{(k)}(\underline{\theta})\underline{g}^{(k)'}(\underline{\theta}) \qquad (2.10)$$

where

$$\bar{t} = (\mu^2\delta - 1)\underline{g}^{(k)}(\underline{\theta}) + \underline{g}^{(k+1)}(\underline{\theta}).$$

2.2.5 The Complementary DFP Updating Formula (CompDFP)

This updating scheme is given by Broyden (1970) and Fletcher (1970), where the formula for the approximate inverse Hessian is given by

$$G^{(k+1)}(\underline{\theta}) = G^{(k)}(\underline{\theta}) + \frac{1}{\underline{p}^{(k)'}\underline{y}^{(k)}}\{\rho\underline{p}^{(k)}\underline{p}^{(k)'} - \underline{p}^{(k)}\underline{y}^{(k)'}G^{(k)}(\underline{\theta})$$

$$- G^{(k)}(\underline{\theta})\underline{y}^{(k)}\underline{p}^{(k)'}\} \qquad (2.11)$$

where

$$\rho = \lambda^{(k)} + \frac{\underline{y}^{(k)'}G^{(k)}(\underline{\theta})\underline{y}^{(k)}}{\underline{p}^{(k)'}\underline{y}^{(k)}}$$

This formula is the complementary DFP formula, that is, when $\underline{y}^{(k)}$ and $\lambda^{(k)}\underline{p}^{(k)}$ are interchanged, equation (2.8) corresponds to the above $G^{(k+1)}(\underline{\theta})$, that is,

$$G^{(k+1)}(\underline{\theta}) = G^{(k)}(\underline{\theta}) + \frac{\underline{y}^{(k)}\underline{y}^{(k)'}}{\lambda^{(k)}\underline{p}^{(k)'}\underline{y}^{(k)}} + \frac{\underline{g}^{(k)}\underline{g}^{(k)'}}{\underline{p}^{(k)'}\underline{g}^{(k)}}$$

The complementary DFP formula in particular has been found to work well in practice, perhaps even better than the DFP formula. It has usually been implemented in conjunction with low accuracy line searches.

2.2.6 Gill-Murray-Pitfield Method (GMP)

In the variable-metric methods which we described in the preceding sections, the approximation $G^{(k+1)}(\underline{\theta})$ to the inverse Hessian of the objective function ϕ at $\underline{\theta}^{(k+1)}$ is obtained by adding either a matrix of rank 1 or a matrix of rank 2 to $G^{(k)}(\underline{\theta})$. But for some k, $G^{(k)}(\underline{\theta})$ may not be positive definite (due to rounding error), so a special method must be employed to ensure that the matrix $G^{(k)}(\underline{\theta})$ is positive definite for all values of k. By resetting $G^{(k)}(\underline{\theta})$ to the unit matrix whenever ϕ cannot be decreased by searching along $\underline{p}^{(k)}$ is not a wholly desirable strategy, because in discarding $G^{(k)}(\underline{\theta})$ we throw away the only knowledge about the curvature of ϕ which is available for use in the algorithm.

However, Gill, Murray and Pitfield (1972) have described an implementation of variable-metric methods which has several advantages over the traditional implementations. In this method, the current estimate of the Hessian matrix is updated, rather than the current estimate $G^{(k)}(\underline{\theta})$ of the inverse Hessian.

(a) The Basic Iteration of GMP

Algorithm 2.5

Step 0: Given $\underline{\theta}^{(k)}$ and $\underline{g}^{(k)}(\underline{\theta})$, calculate $\underline{p}^{(k)}$ by solving the set of equations

$$H^{(k)}\underline{p}^{(k)} = -\underline{g}^{(k)}(\underline{\theta}).$$

The matrix $H^{(k)}$ is recurred in the form

$$H^{(k)} = L^{(k)}D^{(k)}L^{(k)'}$$

where $L^{(k)}$ is a unit-lower triangular matrix, and $D^{(k)}$ a diagonal matrix. The vector $\underline{p}^{(k)}$ can be found by solving successively

$$L^{(k)}\underline{V} = -\underline{g}^{(k)}(\underline{\theta})$$

and

$$L^{(k)\prime}\underline{p}^{(k)} = D^{(k)^{-1}}\underline{V}$$

More explicitly, we have

$$v_i = -g_i^{(k)}(\underline{\theta}) - \sum_{j=1}^{i-1} \ell_{ij}^{(k)} v_j,$$

and

$$p_i^{(k)} = v_i/d_i^{(k)} - \sum_{j=j+1}^{n} \ell_{ji}^{(k)} p_j^{(k)}$$

which require n^2 multiplications and n divisions..

Step 1: Set $\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}$

and

$$\underline{g}^{(k+1)}(\underline{\theta}) = \underline{g}\,(\underline{\theta}^{(k+1)})$$

and $\lambda^{(k)}$ is a scalar such that

$$\phi(\underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}) = \min_{\lambda} \phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)}).$$

Step 2: Modify the triangular factors of $H^{(k)}$ so that

$$H^{(k+1)} = H^{(k)} + \Pi_1 z^{(k)} z^{(k)\prime} + \Pi_2 \omega^{(k)} \omega^{(k)\prime}$$

where $z^{(k)}$, $\omega^{(k)}$ are $n \times 1$ vectors and Π_1, Π_2 are scalars.

Consquently, this revised algorithm uses a formula similar to the recurrence formula (2.10).

(b) Maintenance of Positive Definiteness

We consider the matrix

$$H^{(k+1)} = H^{(k)} + \sigma z^{(k)} z^{(k)'}$$

where σ is a scalar and $z^{(k)}$ an $n \times 1$ column vector. The modification to the Cholesky factorisation (Appendix A) is performed as follows:

Rewrite the above equation as

$$H^{(k+1)} = L^{(k)} D^{(k)\frac{1}{2}} (I + VV') D^{(k)\frac{1}{2}} L^{(k)'} \tag{2.12}$$

where

$$L^{(k)} D^{(k)\frac{1}{2}} V = z^{(k)}$$

Equation (2.12) is then factorised into the form

$$H^{(k+1)} = L^{(k)} D^{(k)\frac{1}{2}} (I - \sigma^{(1)} VV')(I - \sigma^{(1)} VV') D^{(k)\frac{1}{2}} L^{(k)'} \tag{2.13}$$

by writing

$$\sigma^{(1)} = - \frac{\sigma}{1 + (1 + V'V)^{\frac{1}{2}}}$$

The matrix $L^{(k)}D^{(k)\frac{1}{2}}(I - \sigma^{(1)}VV')$ is factorised into the product of a lower triangular and an orthogonal matrix. If $H^{(k+1)}$ is indefinite, $\sigma^{(1)}$ is not real, and $H^{(k+1)}$ must be replaced by a positive definite matrix $\bar{H}$ to guarantee a downhill direction of search. $\bar{H}$ is obtained by redefining $\sigma^{(1)}$ as

$$\sigma^{(1)} = \frac{-\sigma}{1 + (1 + |\sigma|\ V'V)^{\frac{1}{2}}}$$

by the nature of factorisation (2.13) (see Appendix A), $\bar{H}$ will be positive definite and this property cannot be affected by cumulative rounding errors (as happened with earlier algorithms).

2.2.7 The BHHH Hessian Approximation

The BHHH (1974) Hessian approximation is based on the fact that for correctly specified models the Hessian matrix of the likelihood function at the minimising value of $\underline{\theta}$ is equal to the variance-covariance matrix of the gradient of the likelihood function. The result can be used to give a computationally efficient approximation based on the information needed to calculate the gradient, avoiding both the third derivatives required by the analytic Hessian and the repeated function evaluations required by numerical approximation. The approximation used is positive definite almost always, and so should not suffer from the errors associated with the inversion of an ill-conditioned matrix. Its drawbacks are:

(i) that its approximation need not be very good in small samples or for misspecified models, and

(ii) that it provides a consistent estimate of the Hessian only at the true value of $\underline{\theta}$, but in so far as the maximum likelihood estimator is consistent, it can be expected for large samples to provide a good approximation in some neighbourhood of the maximum likelihood estimate.

The BHHH method is an example of a general class (the Gauss-Newton class) of optimisation methods which make use of the statistical properties of the likelihood function and its derivatives. Briefly, at the k^{th} iteration, the BHHH Hessian matrix is approximated by

$$H^{(k)}(\underline{\theta}) = \left[\frac{1}{T}\left(\frac{\partial\phi}{\partial\underline{\theta}}\right)\left(\frac{\partial\phi}{\partial\underline{\theta}}\right)'\right]_{\underline{\theta}^{(k)}}$$

where T is the sample size and $\underline{\theta}^{(k)}$ is the current estimate of the true value $\bar{\underline{\theta}}$. Let $\underline{g}^{(k)}(\underline{\theta}) = \left.\left(\frac{\partial\phi}{\partial\underline{\theta}}\right)\right]_{\underline{\theta}^{(k)}}$, then the iterative algorithm is:

$$\frac{1}{T}\left[\left(\frac{\partial\phi}{\partial\underline{\theta}}\right)\left(\frac{\partial\phi}{\partial\underline{\theta}}\right)'\right]\Delta\,\underline{\theta}^{(k)} - \lambda^{(k)}\left(\frac{\partial\phi}{\partial\underline{\theta}}\right) = 0$$

and the basic Newton step becomes:

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} + \lambda^{(k)}\left[\left.(H^{(k)}(\underline{\theta}))^{-1}\,\underline{g}^{(k)}(\underline{\theta})\right]_{\underline{\theta}=\underline{\theta}^{(k)}}\right]$$

$$= \underline{\theta}^{(k)} + \lambda^{(k)}\,\underline{p}^{(k)}$$

A detailed description of the BHHH method and algorithm is given in Chapter 3.

2.3 Minimisation Without Derivatives

We now describe the two most common optimisation techniques for minimisation without derivatives, and also discuss the disadvantages of such methods in our optimisation problem.

2.3.1 Conjugate Direction Methods

In order to define conjugate directions clearly, we begin by supposing that $\phi(\underline{\theta})$ is a homogeneous positive definite quadratic function, whose second derivative matrix is $H(\underline{\theta})$. Then the n non-zero directions $\underline{p}_i$ $(i = 1, 2, \ldots, n)$ are mutually conjugate if and only if the equations

$$\underline{p}_i' H(\underline{\theta}) \underline{p}_j = 0 , \qquad i \neq j \tag{2.14}$$

hold.

Conjugate directions are important to minimisation algorithms, because, in the above quadratic case, the following construction calculates one vector of variables that minimises $\phi(\underline{\theta})$. Let $\underline{\theta}_o$ be any starting vector. For $i = 1, 2, \ldots, n$, we let $\underline{\theta}_i$ be the vector

$$\underline{\theta}_i = \underline{\theta}_{i-1} + \lambda_{(i)} \underline{p}_i , \tag{2.15}$$

where $\lambda_{(i)}$ is the value of λ that minimises the function of that variable

$$F_i(\lambda) = \phi(\underline{\theta}_{i-1} + \lambda \underline{p}_i) . \tag{2.16}$$

Then $\underline{\theta}_n$ is the point at which $\phi(\underline{\theta})$ is least.

In a conjugate direction method for minimising a general function without calculating derivatives, we begin the k^{th} iteration at the point $\underline{\theta}^{(k)}$, with search directions $\underline{p}_i^{(k)}$ $(i = 1, 2, \ldots, n)$. Initially these directions are the co-ordinate directions, but they are modified on each iteration by some method that should tend to make them mutually conjugate with respect to the Hessian matrix at the solution, $\underline{\theta}^*$ say. The main operation of the k^{th} iteration is to let $\underline{\theta}_o^{(k)} = \underline{\theta}^{(k)}$, and for $i = 1, 2, \ldots, n$ to define $\underline{\theta}_i^{(k)}$ to be the point

$$\underline{\theta}_i^{(k)} = \underline{\theta}_{i-1}^{(k)} + \lambda_i^{(k)} \underline{p}_i^{(k)}, \qquad (2.17)$$

where again $\lambda_i^{(k)}$ is determined by a line search to minimise $\phi(\underline{\theta}_i^{(k)} + \lambda \underline{p}_i^{(k)})$ with respect to λ. We then set $\underline{\theta}^{(k+1)} = \underline{\theta}_n^{(k)}$. Thus if $\underline{\theta}^{(k)}$ is close to $\underline{\theta}^*$, and if the search directions are almost mutually conjugate, we expect $\underline{\theta}^{(k+1)}$ to be much better than $\underline{\theta}^{(k)}$ as an estimate of $\underline{\theta}^*$. However, this description omits the steps required to modify the $\underline{p}_i^{(k)}$. To do this the k^{th} iteration obtains the directions $\underline{p}_i^{(k+1)}$ $(i = 1, 2, \ldots, n)$, which may involve some more values of the objective function. Then a few extra function values may be needed to fix $\underline{\theta}^{(k+1)}$. Usually the value of $\phi(\underline{\theta}^{(k+1)})$ is the least calculated value of the objective function, and always satisfies the inequality $\phi(\underline{\theta}^{(k+1)}) \leqslant \phi(\underline{\theta}^{(k)})$.

For example, most versions of Powell's (1964) algorithm use the formulae

$$\underline{p}_i^{(k+1)} = \underline{p}_{i+1}^{(k)}, \qquad i = 1, 2, \ldots, n-1$$

$$\underline{p}_n^{(k+1)} = \sum_{i=1}^{n} \lambda_i^{(k)} \underline{p}_i^{(k)}, \qquad (2.18)$$

and $\underline{\theta}^{(k+1)}$ is obtained by a line search from $\underline{\theta}_n^{(k)}$ in the direction $\underline{p}_n^{(k+1)}$. Provided $\lambda_1^{(k)}$ is non-zero for all values of k, it may be proved that this method obtains the least value of a quadratic function in at most n iterations.

The conjugate direction methods avoid the two main drawbacks of the variable-metric methods, for they do not require values of $\underline{g}^{(k)}(\underline{\theta})$ $(k = 1, 2, \ldots)$, and most function values are applied to reducing the objective function. However, they too have some disadvantages.

One is that it is sometimes awkward to ensure that for all k the directions $\underline{p}_i^{(k)}$ $(i = 1, 2, \ldots, n)$ have good linear independence properties. For example, if $\lambda_1^{(k)}$ is small in comparison with $\lambda_i^{(k)}$ $(i = 2, 3, \ldots, n)$, then equation (2.18) requires modification. In this case Powell's (1964) algorithm makes the search direction $\underline{p}_n^{(k+1)}$ equal to $\underline{p}_1^{(k)}$, although this change weakens the quadratic termination properties of the method, which often loses efficiency, particularly when n is greater than about ten.

To avoid this difficulty, Brent (1973) suggests a different modification to Powell's algorithm, which requires the eigenvalues and eigenvectors of an $n \times n$ symmetric matrix to be calculated after every n iterations. The extra work of the eigen problems can cause the total computing time to be greater than before, if each evaluation of $\phi(\underline{\theta})$ requires comparatively little time. However, it usually gives a worthwhile reduction in the number of function values needed for the whole minimisation calculation, so Brent's method is recommended for serious problems, where the calculation of $\phi(\underline{\theta})$ is quite long.

Another disadvantage is that conjugate directions may not be well-determined for certain non-quadratic functions. For such ill-conditioned functions, if the second derivative matrix of $\phi(\underline{\theta})$ at certain points is almost singular, it is usual to have a line of such points near the bottom of a curved valley. Therefore it is calamitous that minimisation algorithms often generate sequences of points $\underline{\theta}^{(k)}$ $(k = 1, 2, \ldots)$ that follow curved valleys. Thus the aim of trying to obtain linearly independent conjugate directions, including search directions which allow moves along the floors of any valley, makes the criterion for the choice of new conjugate directions ambiguous. These remarks make the justification for conjugate direction methods with such difficult functions rather uncertain, except in regions of $\underline{\theta}$-space where $\phi(\underline{\theta})$ satisfies a strict convexity condition.

2.3.2 Variable-Metric Methods

The other optimisation technique for minimisation without derivatives is that developed by Gill-Murray-Pitfield (GMP), this method is essentially the same as that of 2.2.6 except for the estimation of the gradient vector. At the beginning of the kth iteration $(k = 1, 2, \ldots)$ of a variable-metric method, we require a starting point $\underline{\theta}^{(k)}$, a vector $\underline{g}^{(k)}(\underline{\theta})$ and a symmetric matrix $H^{(k)}(\underline{\theta})$. The vector $\underline{g}^{(k)}(\underline{\theta})$ is an estimate of the gradient of $\phi(\underline{\theta})$ at $\underline{\theta}^{(k)}$, and the matrix $H^{(k)}(\underline{\theta})$ is an estimate of the Hessian matrix of $\phi(\underline{\theta})$ at $\underline{\theta}^{(k)}$.

Sometimes the errors in $H^{(k)}(\underline{\theta})$ are quite large. For example, in many useful algorithms it is advantageous to force $H^{(k)}(\underline{\theta})$ to be positive definite, even though the true second derivatives may have negative eigenvalues at $\underline{\theta}^{(k)}$. To simplify the description, we suppose in this section that $H^{(k)}(\underline{\theta})$ is positive definite on every iteration.

The derivative estimates provide the quadratic approximation

$$\phi(\underline{\theta}^{(k)} + \underline{\delta}) \simeq \phi(\underline{\theta}^{(k)}) + \underline{\delta}'\underline{g}^{(k)}(\underline{\theta}) + \frac{1}{2}\,\underline{\delta}'H^{(k)}(\underline{\theta})\,\underline{\delta} \qquad (2.19)$$

The value of $\underline{\delta}$ that minimises the right-hand side of (2.19) satisfies the equation

$$\underline{g}^{(k)}(\underline{\theta}) + H^{(k)}(\underline{\theta})\underline{\delta} = 0 \tag{2.20}$$

Therefore some variable-metric methods define $\theta^{(k+1)}$ by the equation

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} - [H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta}). \tag{2.21}$$

However, because this choice of $\underline{\theta}^{(k+1)}$ may conflict with inequality $\phi(\underline{\theta}^{(k+1)}) \leq \phi(\underline{\theta}^{(k)})$, it is usual to let $\underline{\theta}^{(k+1)}$ be the vector

$$\underline{\theta}^{(k+1)} = \underline{\theta}^{(k)} - \lambda^{(k)}[H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta}) \tag{2.22}$$

where $\lambda^{(k)}$ is a scalar which is chosen to enforce the above condition, and possibly another condition also to ensure that $H^{(k+1)}(\underline{\theta})$ is positive definite. To determine the value of $\lambda^{(k)}$, we seek a good estimate of the least value of the function

$$F(\lambda) = \phi(\underline{\theta}^{(k)} - \lambda[H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta})) \tag{2.23}$$

by calculating only a few actual values of $F(\lambda)$. A description of a suitable method for adjusting λ is given in section 2.4.

Next the gradient of $\phi(\underline{\theta})$ at the point $\underline{\theta}^{(k+1)}$ is estimated. Usually in non-derivative algorithms, either forward or central differences are employed, the i^{th} component of $\underline{g}^{(k+1)}(\underline{\theta})$ $(i = 1, 2, \ldots)$ being defined by the equation

$$g_i^{(k+1)}(\theta) = \{\phi(\underline{\theta}^{(k+1)} + h_i\underline{e}_i) - \phi(\underline{\theta}^{(k+1)})\}/h_i \tag{2.24}$$

or by the equation

$$g_i^{(k+1)}(\theta) = \{\phi(\underline{\theta}^{(k+1)} + h_i\underline{e}_i) - \phi(\underline{\theta}^{(k+1)} - h_i\underline{e}_i)\}/2h_i, \quad (2.25)$$

where $\underline{e}_i$ is the i^{th} co-ordinate vector.

An important and valuable feature of the methods used to define $H^{(k+1)}(\underline{\theta})$ is that they require no more values of the objective function. The successful choices of $H^{(k+1)}(\underline{\theta})$ satisfy the equation

$$H^{(k+1)}(\underline{\theta})[\underline{\theta}^{(k+1)} - \underline{\theta}^{(k)}] = [\underline{g}^{(k+1)}(\underline{\theta}) - \underline{g}^{(k)}(\underline{\theta})] \quad (2.26)$$

because, when $\phi(\underline{\theta})$ is a quadratic function, this equation is also satisfied by the true Hessian matrix. One of the most useful choices of $H^{(k+1)}(\underline{\theta})$ is that given by the Broyden-Fletcher-Shanno formula

$$H^{(k+1)}(\underline{\theta}) = H^{(k)}(\underline{\theta}) - \frac{H^{(k)}(\underline{\theta})\underline{\delta}^{(k)}\underline{\delta}^{(k)'}H^{(k)}(\underline{\theta})}{\underline{\delta}^{(k)'}H^{(k)}(\underline{\theta})\underline{\delta}^{(k)}} + \frac{\underline{\gamma}^{(k)}\underline{\gamma}^{(k)'}}{\underline{\gamma}^{(k)'}\underline{\delta}^{(k)}}, \quad (2.27)$$

where $\underline{\delta}^{(k)}$ and $\underline{\gamma}^{(k)}$ are the differences

$$\underline{\delta}^{(k)} = \underline{\theta}^{(k+1)} - \underline{\theta}^{(k)},$$
$$\underline{\gamma}^{(k)} = \underline{g}^{(k+1)}(\underline{\theta}) - \underline{g}^{(k)}(\underline{\theta}). \quad (2.28)$$

Thus the data that is needed to begin the next iteration is already calculated.

The extensive numerical results given by Gill-Murray-Pitfield (1972) indicate that the class of variable-metric methods contains the best of the available algorithms for minimisation without derivatives. However, each iteration of a variable-metric method uses at least n function values to estimate first derivatives, but it uses only about three or four function values in the line search that seeks the minimum of the function (2.23). Thus in large problems only a small proportion of the function evaluations are applied directly to the main problem of reducing the objective function. This is a poor strategy unless $\phi(\underline{\theta})$ is almost quadratic.

Another deficiency of variable-metric methods is that usually the search direction $-[H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta})$ in expression (2.22) gives fast convergence only if the direction of $\underline{g}^{(k)}(\underline{\theta})$ is a good approximation to the direction of the true gradient of $\phi(\underline{\theta})$ at $\underline{\theta}^{(k)}$. However, the true gradient should tend to zero as k increases, so the difficulties of calculating a suitable vector $\underline{g}^{(k)}(\underline{\theta})$ become more and more severe. Therefore many algorithms switch from formula (2.24) to formula (2.25) when $\underline{g}^{(k)}(\underline{\theta})$ becomes small, in order to obtain higher accuracy at the cost of almost doubling the number of function values per iteration. Thus the precision of the calculated values of $\phi(\underline{\theta})$ is very important. To avoid these extra function values, Cullum (1972) suggest the formula

$$g_i^{(k+1)} = \{\phi(\underline{\theta}^{(k+1)} + h_i\underline{e}_i) - \phi(\underline{\theta}^{(k+1)}) - \tfrac{1}{2}h_i^2H_{ii}^{(k)}(\underline{\theta})\}/h_i \qquad (2.29)$$

instead of equation (2.25), where $H_{ii}^{(k)}(\underline{\theta})$ is the i^{th} diagonal element of $H^{(k)}(\underline{\theta})$.

Another way of obtaining better accuracy in the differences (2.24) and (2.25) is to avoid the use of adaptive methods in the calculation of $\phi(\underline{\theta})$. For example, if $\phi(\underline{\theta})$ is a definite integral which is calculated by a numerical quadrature formula, and if the weights of the quadrature formula are held constant, then the leading error term of the quadrature formula usually cancels out when the difference (2.24) or (2.25) is formed.

The choice of the step-length h_i in equation (2.24) and (2.25) also causes problems. The earliest variable-metric method (Stewart, 1967) includes a technique that chooses h_i automatically, and numerical results show that it works quite well. However, Gill and Murray (1972) suggest that it is better to keep h_i $(i = 1, 2, \ldots, n)$ constant throughout the calculation, in order that the leading error terms in $\underline{g}^{(k)}(\underline{\theta})$ and $\underline{g}^{(k+1)}(\underline{\theta})$ cancel when $\underline{\gamma}^{(k)}$ is calculated from expression (2.28). In our opinion, it is preferable if the step-lengths are adjusted automatically, so that people who do not understand the difficulties of numerical differentiation can apply the minimisation subroutines successfully, without expert advice on the choice of h_i.

2.3.3 Comments Regarding Minimisation Without Derivatives

Although the most successful algorithms now for minimisation without derivatives are variable-metric and conjugate direction methods, we have noted major disadvantages in both these classes of methods. Difficulties occur in variable-metric methods because of the strong dependence on accurate first derivatives, and in conjugate direction methods the revision of the conjugate directions can be a very poorly defined problem. However, the estimation of second derivatives in a variable-metric method seldom impairs efficiency, and the fact that conjugate direction methods usually search along n independent directions on every iteration helps to avoid jamming away from the solution. But finding a good algorithm which may retain the advantages and lose the disadvantages of current algorithms may take a long time, particularly because comparisons should be made with current methods that have been designed and programmed carefully. Therefore, in this study, we concentrate our effort on minimisation methods with analytic derivatives, and we will implement the BHHH and GMP methods in our computer program to estimate the parameters of the concentrated log-likelihood function.

2.4 Choice of Line Search

An important part of all these minimisation algorithms is the choice of the step-length $\lambda^{(k)}$ along the direction $\underline{p}^{(k)}$.

Although some algorithms have been suggested which generally accept $\lambda^{(k)} = 1$, it is usual to require that $\lambda^{(k)}$ is chosen to ensure that $\phi(\underline{\theta}^{(k+1)}) \leq \phi(\underline{\theta}^{(k)})$, which gives a minimal stability in the iteration. Although it may cost relatively little in computing time to ensure that $\lambda^{(k)}$ is chosen so as to minimise

$$\phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)}),$$

this may be relatively wasteful of computer time when the cost of computing $\phi(\underline{\theta})$ is high, or if n is so large that in the early iterations, when the direction $\underline{p}^{(k)}$ is relatively arbitrary, there is no great advantage in searching along the direction $\underline{p}^{(k)}$. It is necessary to balance the time taken in searching along the direction $\underline{p}^{(k)}$ with the time taken to choose a more suitable direction $\underline{p}^{(k+1)}$. This balance is clearly dependent on the properties of the function $\phi(\underline{\theta})$, and is usally decided on the basis of experience with a variety of functions.

2.4.1 Quadratic Interpolation

Powell (1964) published a simple algorithm for determining the minimising value of λ, using quadratic interpolation. This algorithm forms part of Powell's more general method of finding the minimum value of a function $\phi(\underline{\theta})$ without calculating derivatives. However, it may also be used in conjunction with any gradient method, or more generally, with any optimisation technique which requires a one-dimensional search.

To find the minimum on a line, we must provide the following:

(i) a set of points (or a point) on the line, $\underline{\theta}$,

(ii) the direction of the line $\underline{p}$,

(iii) an upper bound to the length of step along the line, m,

(iv) an order of magnitude of the length of step along the line, h, assumed to be less than m, and

(v) the accuracy to which the minimum is required, ε.

The method of minimisation must be such as to find the minimum of a quadratic form, so it is primarily based on the quadratic defined by three function values.

Initially $\phi(\underline{\theta})$ and $\phi(\underline{\theta} + h\underline{p})$ are calculated, and then either $\phi(\underline{\theta} - h\underline{p})$ or $\phi(\underline{\theta} + 2h\underline{p})$ is worked out depending on whether $\phi(\underline{\theta})$ is less than or greater than $\phi(\underline{\theta} + h\underline{p})$. These three function values are now used in the general formula which predicts the turning value of the quadratic defined by $\{a, \phi(\underline{\theta} + a\underline{p})\}$, $\{b, \phi(\underline{\theta} + b\underline{p})\}$, and $\{c, \phi(\underline{\theta} + c\underline{p})\}$ to be at $(\underline{\theta} + \lambda\underline{p})$, where

$$\lambda = \frac{1}{2} \cdot \frac{(b^2 - c^2)\phi_a + (c^2 - a^2)\phi_b + (a^2 - b^2)\phi_c}{(b - c)\phi_a + (c - a)\phi_b + (a - b)\phi_c} . \tag{2.30}$$

It is a minimum if

$$\frac{(b - c)\phi_a + (c - a)\phi_b + (a - b)\phi_c}{(a - b)(b - c)(c - a)} < 0. \tag{2.31}$$

If the turning value is predicted to be a maximum, or if the value of λ is such that to calculate $\phi(\underline{\theta} + \lambda \underline{p})$ a step greater than m must be taken, the maximum allowed step is taken in the direction of decreasing ϕ, and the function value at the point which is furthest from $(\underline{\phi} + \lambda \underline{p})$ is discarded, so the prediction may be repeated.

Otherwise λ is compared with a, b, c, and, if it is within the required accuracy of one of them, that point is chosen as the minimum. If it is not, $\phi(\underline{\theta} + \lambda \underline{p})$ is calculated so that the quadratic prediction may be repeated; the function value which is thrown away out of $\phi(\underline{\theta} + a\underline{p})$, $\phi(\underline{\theta} + b\underline{p})$ and $\phi(\underline{\theta} + c\underline{p})$ is normally the greatest, but it is not if rejecting a smaller one can yield a definite bracket on a minimum, which would not be obtained otherwise.

In order to reduce the number of times $\phi(\theta_1, \theta_2, \ldots, \theta_n)$ has to be calculated, advantage may be taken of the fact that three function values are sufficient to predict

$$\frac{\partial^2}{\partial \lambda^{*2}} \{\phi(\underline{\theta} + \lambda^* \underline{p})\}. \tag{2.32}$$

The prediction of the second derivative is

$$\zeta = -2 \cdot \frac{(b-c)\phi_a + (c-a)\phi_b + (a-b)\phi_c}{(a-b)(b-c)(c-a)} \qquad (2.33)$$

So, if after finding the minimum in the direction $\underline{p}$ the components of $\underline{p}$ are scaled by $1/\sqrt{\zeta}$, the next time a minimum is sought in the same direction the unit second derivative may be used. In this case just $\phi(\underline{\theta})$ and $\phi(\underline{\theta} + h\underline{p})$ are sufficient to predict the minimum to be at $(\underline{\theta} + \lambda\underline{p})$,

$$\lambda = \frac{1}{2}h - \frac{\phi(\underline{\theta} + h\underline{p}) - \phi(\underline{\theta})}{h} . \qquad (2.34)$$

<u>Choice of h</u>

It is important to have a method of adjusting the step-length h before entering the line search procedure to ensure that a definite bracket on a minimum is located without too many function evaluations. Assume we have the initial step $\lambda = 1$, and during each iteration a new step λ^* is obtained, we can then set

$$D = ||P||_2 * \lambda^*$$

and define

$$\lambda = \min\{\max(\lambda/2, 2D), 2\lambda\}$$

that is,

if $\lambda > D \geq \lambda/4$, reset $\lambda_1 = 2D$,

if $\lambda/4 \geq D$, reset $\lambda_1 = \lambda/2$.

This will ensure that $\lambda/2 \leq \lambda_1 \leq 2\lambda$.

We then set

$$h = \min (1, \lambda_1 / \|p\|_2)$$

as our starting step-length in the line search algorithm.

A simple method for choosing h is described in the following steps:

Within the optimisation routine: ($\lambda = 1$, is assumed initially)

1. Compute $d = \|\underline{p}\|_2$.
2. Set $h = \min (1, \lambda/d)$.
3. Call line search to locate a new step-length λ^*.
4. Compute $D = d * \lambda^*$.
5. Reset $\lambda = \min\{\max (\lambda/2, 2D), 2\lambda\}$.
6. Return to the optimisation routine.

Consequently, our estimation program for the non-linear econometric system uses the above procedures for the line search and adjusting the step-length h.

2.4.2 Cubic Interpolation

The line search given in the GMP procedure is that suggested by Davidon (1959). Given two points λ_1 and λ_2 with function values ϕ_1 and ϕ_2 and derivatives $\underline{g}_1 = \underline{g}(\underline{\theta}^{(1)})$ and $\underline{g}_2 = \underline{g}(\underline{\theta}^{(2)})$, a stationary point λ^* of the third order polynomial passing through these two points and having the specified derivative values is given by

$$\lambda^* = (\lambda_2 - \lambda_1)(1 - (\underline{g}_2 - \gamma - \eta)/(\underline{g}_2 - \underline{g}_1 + 2\gamma)) \qquad (2.35)$$

where

$$\gamma = (\eta^2 - \underline{g}_1\underline{g}_2)^{\frac{1}{2}}$$

and

$$\eta = 3(\phi_1 - \phi_2)/(\lambda_2 - \lambda_1) + \underline{g}_1 + \underline{g}_2.$$

The stationary point defined above is the one which lies in the interval (λ_1, λ_2) if the minimum of $\phi(\underline{\theta})$ along $\underline{p}^{(k)}$ lies in this interval. Assuming $\lambda_1 < \lambda_2$ then the minimum lies in the interval (λ_1, λ_2) if $\underline{g}_1 < 0$ and $\underline{g}_2 > 0$.

In the non-derivative case, quadratic interpolation is applied. The stationary point λ^* of the second order polynomial passing through three points is given by equation (2.30).

2.4.3 Bard Line Search

An alternative method of choosing $\lambda^{(k)}$ is given by Bard (1970).

Define

$$F_k(\lambda) \equiv \phi(\underline{\theta}^{(k)} + \lambda[H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta})),$$

where $\underline{g}^{(k)}(\underline{\theta})$ is the gradient vector and $H^{(k)}(\underline{\theta})$ is the approximate Hessian matrix,

$$\lambda_{max} \equiv \text{upper bound on } \lambda_i.$$

Bard considers the case where there are inequality constraints and in this case, λ_{max} is determined as the minimum positive λ such that $\underline{\theta} + \lambda[H(\underline{\theta})]^{-1}\underline{g}(\underline{\theta})$ is on a constraint.

When there is no inequality, λ_{max} is set to an arbitrary large number.

At the start of the k^{th} iteration, we possess the value

$$F_k(0) = \phi(\underline{\theta}^{(k)})$$

and

$$F_k'(0) \equiv \left.\frac{dF_K}{d\lambda}\right|_{\lambda=0} = \underline{g}^{(k)'}(\underline{\theta})[H^{(k)}(\underline{\theta})]^{-1}\underline{g}^{(k)}(\underline{\theta}).$$

$\lambda^{(o)}$ is assumed given at the start of the k^{th} iteration and define $F^{(o)} = F_k(\lambda^{(o)})$.

<u>The Basic Algorithm</u>

Step 0: Compute $F^{(o)}$. If $F^{(o)} < F_k(o)$ accept $\lambda^{(k)} = \lambda^{(o)}$, otherwise continue.

Step 1: Determine the second degree polynomial in λ which agrees with $F_k(\lambda)$ at $\lambda = 0$ and $\lambda = \lambda^{(o)}$, and whose slope at $\lambda = 0$ agrees with $F_k'(0)$. Let $\lambda^{(1)}$ be the point at which this polynomial is stationary, that is, define

$$F_k^*(\lambda) = F_k(0) + F_k'(0)\lambda + \alpha\lambda^2$$

where α is chosen so that

$$F_k(\lambda^{(o)}) = F_k(0) + F_k'(0)\lambda^{(o)} + \alpha\lambda^{(o)2}.$$

Then we have

$$\alpha = \frac{F_k(\lambda^{(o)}) - F_k(0) - F_k'(0)\lambda^{(o)}}{\lambda^{(o)2}}.$$

The stationary value is given by

$$F_k'(0) + 2\alpha\lambda = 0, \text{ and}$$

$$\lambda^{(1)} = -\frac{F_k'(0)}{2\alpha}$$

$$= -\frac{F_k'(0)\lambda^{(o)2}}{2\{F_k(\lambda^{(o)}) - F_k(0) - F_k'(0)\lambda^{(o)}\}}$$

Step 2: If this is the first $\lambda^{(1)}$ calculated for the k^{th} iteration go to Step 3, otherwise define

$$\lambda^{(2)} \equiv \max[\,0.25\lambda^{(o)},\ \min(0.75\lambda^{(o)},\ \lambda^{(1)})],$$

that is, if $0.25\lambda^{(o)} < \lambda^{(1)} < 0.75\lambda^{(o)}$, set $\lambda^{(2)} = \lambda^{(1)}$

if $\lambda^{(1)} > 0.75\lambda^{(o)}$, set $\lambda^{(2)} = 0.75\lambda^{(o)}$

if $\lambda^{(1)} < 0.25\lambda^{(o)}$, set $\lambda^{(2)} = 0.25\lambda^{(o)}$

Replace $\lambda^{(o)}$ with $\lambda^{(2)}$ and return to Step O.

Step 3: Define $\lambda^{(3)} \equiv \min(\lambda^{(1)}, 0.75\lambda_{max})$.

Step 4: If $|\lambda^{(3)} - \lambda^{(o)}| \leq 0.1\lambda^{(o)}$ or $\lambda^{(1)} \leq 0.25\lambda^{(o)}$, accept $\lambda^{(k)} = \lambda^{(o)}$, otherwise continue.

Step 5: Compute $F^{(3)} = F_k(\lambda^{(3)})$. Take $\lambda^{(k)} = \lambda^{(3)}$ or $\lambda^{(k)} = \lambda^{(o)}$ depending on whether $F^{(3)}$ or $F^{(o)}$ is the smaller.
Bard line search is different from other methods because it considers the problem whether $\phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)})$ is on a constraint.

2.4.4 The BHHH Line Search

To choose $\lambda^{(k)}$, Berndt-Hall-Hall-Hausman (1974) suggest that an arbitrary δ is chosen, $0 < \delta < \frac{1}{2}$.

The BHHH procedure is then to take $\lambda = 1$ if

$$\phi(\underline{\theta}^{(k)} + \underline{p}^{(k)}) - \phi(\underline{\theta}^{(k)}) \geq \delta\underline{p}^{(k)'}\underline{g}^{(k)}(\underline{\theta}) \qquad (2.36)$$

and otherwise choose $\lambda^{(k)}$ such that

$$\delta\lambda^{(k)}\underline{p}^{(k)'}\underline{g}^{(k)}(\underline{\theta}) \leq \phi(\underline{\theta}^{(k)} + \lambda^{(k)}\underline{p}^{(k)}) - \phi(\underline{\theta}^{(k)})$$

$$\leq (1-\delta)\lambda^{(k)}\underline{p}^{(k)'}\underline{g}^{(k)}(\underline{\theta}). \qquad (2.37)$$

Now if condition (2.36) is not satisfied,

$$\phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)}) - \phi(\underline{\theta}^{(k)}) < \delta\lambda\underline{p}^{(k)'}\underline{g}^{(k)}(\underline{\theta})$$

for λ just less than 1, and

$$\{\phi(\underline{\theta}^{(k)} + \lambda\underline{p}^{(k)}) - \phi(\underline{\theta}^{(k)})\}/\lambda\underline{p}^{(k)'}\underline{g}^{(k)}(\underline{\theta}) \to 1 \quad \text{as} \quad \lambda \to 0.$$

Thus by reducing λ from 1, we can find a $\lambda^{(k)}$ satisfying equation (2.37). Unfortunately this may be a time-wasting procedure, since we often find that it is necessary to consider several values of λ before a suitable $\lambda^{(k)}$ is found.

2.4.5 Efficiency and Termination

The four possible line search procedures have been programmed. Each of these has been tested in separate runs on a set of simulated non-linear simultaneous models.

From the results, it became clear that procedures Bard and BHHH are relatively time-wasting compared with quadratic and cubic interpolations because we have to compute several λ_i before we can locate a suitable $\lambda^{(k)}$. It is expensive in terms of computing time to compute many function evaluations as the objective function ϕ can be very complex. These extra function values required in each line search are not compensated for by finding a lower value of $F(\lambda)$, nor do the theoretically better convergence properties show up in our comparisons. Hence more iterations are needed in the iterative procedures for the model to achieve convergence.

Cubic interpolation again has a drawback because it is relatively expensive to compute the gradient of ϕ at λ_2, but it is a more efficient method compared with Bard and BHHH.

We would recommend the use of quadratic interpolation as a line search procedure. Since the step-length h is adjusted during each iteration, we have a good projection of $\lambda^{(k)}$ for a start and hence reduce the possibility of searching too many λ_i on the line $\phi(\underline{\theta} + \lambda_i \underline{p})$. The average number of function evaluations in this procedure is between 1 to 2. Since we can locate a good estimate of $\lambda^{(k)}$ with a smaller number of function evaluations, we are not only reducing the computing time for function evaluations, but also the time taken to optimise the model.

2.5. Choice of Stopping Criterion

Determining when to stop the iterations that lead to a minimum of ϕ is a problem of great practical interest: stopping short of the mark has its obvious costs in the quality of the estimates; going too far involves unecessary costs in computer time.

2.5.1 The Gradient Stopping Criterion

In principle there seems little problem determing when to stop: at the minimum the gradient is zero. Thus it is common practice to choose some arbitrarily small ε, such as 10^{-4} or 10^{-5}, and to stop when the largest gradient (in absolute value) is less than ε. This stopping criterion, called the gradient criterion, can also be effected by stopping when the square length of $\underset{\sim}{g}$ (where $\underset{\sim}{g} = \underset{\sim}{g}^{(k)}(\underline{\theta})$) is small, that is, when

$$\|\underset{\sim}{g}\|_2 \leq \varepsilon .$$

The gradient criterion has two major weaknesses. First, it is scale-sensitive. Changes in the units in which the data are measured can cause the scale of specific parameters and their gradients to be made arbitrarily large or small. In econometric problems, parameters that are naturally small will tend to have relatively large gradients that can keep the optimiser seeking a minimum long after it is close enough for practical purposes. Similarly, large coefficients (some constant terms) may have relatively small gradients that can be ignored by this criterion even when they should not be. In practice, the gradient stopping criterion is very conservative, tending to drive the optimiser beyond the point of diminishing returns in terms of parameter estimates. It tends, therefore, to be a good criterion when we wish to be sure to go far enough.

A second weakness of the gradient criterion is that it ignores the statistical context of likelihood estimation and treats all parameters alike - whether they are significant or not. It is quite possible for a large gradient in the direction of a wholly insignificant parameter estimate to force the continuation of the optimisation process even though those parameters that are estimated with significance are changing little.

2.5.2 The Weighted-Gradient Stopping Criterion

Here the weighted-gradient stopping criterion is introduced, that is,

$$- \underline{g}'H^{-1}\underline{g} \leq \varepsilon, \qquad \text{where} \quad H = H^{(k)}(\underline{\theta}).$$

This criterion equals zero (assuming H^{-1} is negative definite) if and only if $\underline{g} = 0$, and it is scale-invariant. If H is ill-conditioned $- \underline{g}'H^{-1}\underline{g}$ could be large even if $\underline{g}$ is small. This characteristic is in fact an advantage of the weighted-gradient criterion in the NLFIML context, for, near the maximum likelihood solution, the negative of the Hessian estimates the variance-covariance matrix of $\underline{g}$. An ill-conditioned Hessian occurs when some element of $\underline{\theta}$ has a high variance and the corresponding element of $\underline{g}$ has a small variance. Thus, this criterion incorporates a weighting scheme that, near the solution, takes into account the precision with which the gradient components are known: gradients with large variances are appropriately downweighted or conversely. Therefore the weighted-gradient criterion would seem to have value as a stopping criterion. However, in practice we found criteria of this kind tended to stop earlier than other criteria, and we preferred to make use of criteria which were not so directly related to the statistical properties of our estimators, but rather to the numerical properties of the errors in the parameters or derivatives.

For our stopping criteria in the estimation program, we would use:

(a) $\|\underline{g}\|_2 < \varepsilon_1$

(b) $$\left|\frac{\theta_i^{(k)} - \theta_i^{(k-1)}}{\theta_i^{(k-1)}}\right| < \varepsilon_2, \forall_i$$

(c) $$\left|\frac{\phi(\underline{\theta}^{(k+1)}) - \phi(\underline{\theta}^{(k)})}{\phi(\underline{\theta}^{(k)})}\right| < \varepsilon_3$$

where ε_1, ε_2 and ε_3 are prescribed tolerance levels. If any two of the above stopping criteria are satisfied, we will then terminate the iterative procedure.

CHAPTER 3

CHARACTERISTICS OF ECONOMETRIC ESTIMATION PROBLEMS

3. The Model

We are concerned with estimation in the multivariate model

$$f_i(y_t; z_t; \theta) \equiv f_i(y_{1t}, \ldots, y_{nt}; z_{1t}, \ldots, z_{mt}; \theta_1, \ldots, \theta_K)$$

$$= u_{it} \qquad i = 1, \ldots, n$$

$$t = 1, \ldots, T \qquad (3.1)$$

where $u_t = (u_{1t}, \ldots, u_{nt})'$ is the vector of normally distributed, serially independent disturbances with mean zero and a symmetric positive definite variance covariance matrix Ω, θ is the vector of K unknown parameters, $f_i(.;.;.)$ is a twice continuously differentiable function, y_t is an $(n \times 1)$ vector of jointly dependent variables and z_t is an $(m \times 1)$ vector of predetermined variables.

We now set up a likelihood function based on a multivariate normal distribution for the u_{it}. Noting that the joint probability density function for u_t is

$$(2\pi)^{-\frac{n}{2}} |\Omega|^{-\frac{1}{2}} \exp\{-\tfrac{1}{2} u_t'\Omega^{-1}u_t\},$$

the joint probability for the T observations $(y_t; z_t; \ t = 1, \ldots, T)$ is:

$$d^nP = (2\pi)^{-\frac{nT}{2}} (\det \Omega)^{-\frac{T}{2}} \left(\prod_{t=1}^{T} |\det J_t|\right) * \exp \{-\frac{1}{2} \sum_{ijt} f_{it} \Omega^{ij} f_{jt}\} dv \tag{3.2}$$

where

$$dv = \prod_{t=1}^{T} (dy_{1t}, dy_{2t}, \ldots, dy_{nt})$$

$$f_{it} = f_i(y_t; z_t; \theta)$$

det J_t is the Jacobian determinant (i.e. the determinant of first derivatives w.r.t. y_t) with

$$J_t = \left[\frac{\partial f_{it}(y_t; z_t; \theta)}{\partial y_{it}}\right] \tag{3.3}$$

and Ω^{ij} is the ij^{th} element of Ω^{-1}. The logarithm of the likelihood is then

$$L(\theta, \Omega) = -\frac{nT}{2} \log 2\pi + \frac{T}{2} \log (\det \Omega^{-1}) + \sum_t \log |\det J_t|$$

$$-\frac{1}{2} \sum_{ijt} f_{it} \Omega^{ij} f_{jt}. \tag{3.4}$$

The Maximum Likelihood (ML) estimator of θ and Ω is implicitly defined as a solution to the following necessary first order conditions for the maximum of the log-liklihood function $L(\theta, \Omega)$:

$$\frac{\partial L(\theta, \Omega)}{\partial \Omega^{ij}} = 0 \qquad \begin{array}{l} i = 1, \ldots, n \\ j = 1, \ldots, i \end{array} \tag{3.5}$$

$$\frac{\partial L(\theta, \Omega)}{\partial \theta_\alpha} = 0 \qquad \alpha = 1, \ldots, K. \tag{3.6}$$

Finding the ML estimator involves solving these equations for $K + n(n+1)/2$ unknown parameters. The dimentionality (and quite possibly the computational expense) of this problem can be reduced considerably by noting that the elements of Ω are unrestricted (except that Ω is symmetric and positive definite). Hence Ω can be eliminated from the log-liklihood function by concentrating it out, that is, by solving the ML estimator of Ω in (3.5) <u>analytically</u> and substituting Ω by its ML estimator in (3.4).

Because Ω^{-1} is symmetric,

$$\frac{\partial \log (\det \Omega^{-1})}{\partial \Omega^{ij}} = \begin{cases} \Omega_{ii} & \text{if } i = j \\ 2\Omega_{ij} & \text{if } i \neq j \end{cases} \tag{3.7a}$$

and so

$$\frac{\partial L(\theta, \Omega)}{\partial \Omega^{ij}} = \begin{cases} \frac{T}{2}\Omega_{ii} - \frac{1}{2}\sum_t f_{it}f_{it} \\ T\Omega_{ij} - \sum_t f_{it}f_{jt} . \end{cases} \tag{3.7b}$$

Setting the derivatives in (3.7b) equal to zero as in (3.5) gives the ML estimator of Ω_{ij} $(i, j = 1, \ldots, n)$:

$$\frac{1}{T}\sum_t f_{it}f_{jt} . \tag{3.8}$$

Upon substituting this into the log-likelihood function in (3.4), the last term of that equation is

$$-\frac{1}{2}\sum_{ijt} f_{it}\Omega^{ij}f_{jt} = -\frac{1}{2}\sum_{ij}\Omega^{ij}\sum_t f_{it}f_{jt} = -\frac{1}{2}\sum_{ij}\Omega^{ij}T\Omega_{ij}$$

$$= -\frac{T}{2}\,\mathrm{tr}(\Omega^{-1}\Omega)$$

$$= -\frac{nT}{2}\,. \qquad (3.9)$$

Hence the last term in equation (3.4) is a constant. The non-constant part of $L(\theta)$ is

$$\frac{T}{2}\log(\det\Omega^{-1}) + \sum_t \log|\det J_t|\,. \qquad (3.10)$$

Thus the concentrated log-likelihood function is

$$L^*(\theta) = c + \sum_t \log|\det J_t| - \frac{T}{2}\log\left(\det\left(\sum_t \frac{f_{it}f_{jt}}{T}\right)\right) \qquad (3.11)$$

where c is the constant $\frac{nT}{2}\log T - \frac{nT}{2}\log(2\pi) - \frac{nT}{2}$. $L^*(\theta)$ is a function of θ only (and not Ω). Further the ML estimator for θ and Ω obtained from (3.5) and (3.6) is identical to that obtained by solving for $\partial L^*(\theta)/\partial\theta_\alpha = 0$ $\alpha = 1, \ldots, K$, and using (3.8) as the ML estimator of Ω_{ij}. Working with the concentrated log-likelihood for $L^*(\theta)$ gives a simple <u>analytic</u> expression for the ML estimator of Ω and reduces the number of parameters which need to be estimated by iterative techniques from $K + n(n+1)/2$ to K, thereby saving on computational costs.

3.1 The BHHH Method of Estimation and Inference by Maximum Likelihood

Maximum likelihood estimates are assumed to be generally statistically efficient in large samples. Berndt-Hall-Hall-Hausman (BHHH, 1974) have developed a practical approach to maximum likelihood estimation within the framework of gradient methods. Their approach has two advantages over the application of Newton's method (Eisenpress and Greenstadt (1966), Chow (1973)). First, its convergence is more likely since unlike Newton's method which uses a Hessian matrix that may not be positive definite, it confines the direction vector to the gradient halfspace. Second, the BHHH method requires the evaluation of derivatives of the functions f_{it} up to second only, while Newton's method requires certain third derivatives of functions f_{it}.

We need to maximise $L^*(\theta)$ the concentrated log-likelihood function defined in equation (3.11).

Differentiating (3.11) w.r.t. θ, the gradient of the log-likelihood function is:

$$\frac{\partial L^*}{\partial \theta} = \sum_t \frac{\partial}{\partial \theta} \log |\det J_t| - \frac{T}{2} \frac{\partial}{\partial \theta} \log \left[\det\left(\sum_t \frac{f_{it} f_{jt}}{T}\right)\right]$$

$$= p - q, \text{ say,} \qquad (3.12)$$

or $$\sum_{t=1}^{T} \frac{\partial L_t^*}{\partial \theta} = \sum_{t=1}^{T} (p_t - q_t).$$

The variance-covariance matrix of the gradient is given by:

$$E\left[\left(\frac{\partial L^*}{\partial \theta}\right)\left(\frac{\partial L^*}{\partial \theta}\right)'\right] = E\left[(p - q)(p - q)'\right]. \tag{3.13}$$

Define

$$\begin{aligned} p_{kt} &= \frac{\partial}{\partial \theta_k} \log \left|\det J_t\right| \\ &= \sum_{i,j} (J_t)^{-1}_{i,j} \frac{\partial J_{t,i,j}}{\partial \theta_k} \end{aligned} \tag{3.14}$$

where $\partial^2 f_t/\partial \theta_k \partial y$ is the square matrix with typical element $\partial^2 f_{ti}/\partial \theta_k \partial y_j$, $i = 1, \ldots, n,$ $j = 1, \ldots, n,$ and

$$q_{ti} = \left(\frac{\partial f_t}{\partial \theta_i}\right)'\left(\sum_{t=1}^{T} \frac{f_{jt} f_{kt}}{T}\right)^{-1} f_t \ . \tag{3.15}$$

Let $Q_t = \dfrac{\partial^2 L^*_t}{\partial \theta \partial \theta'}$ and

$$Q = \sum_{t=1}^{T} Q_t , \quad \bar{Q} = T^{-1} Q.$$

Then

$$\bar{Q}_{\bar{\theta}} = \frac{1}{T}\left(\frac{\partial^2 L^*}{\partial \theta \partial \theta'}\right)_{\theta=\bar{\theta}}$$

where $\bar{\theta}$ is the true value of θ, has the property

$$E\left(\bar{Q}_{\bar{\theta}}\right) = -E\left(\frac{1}{T}\left(\frac{\partial L^*}{\partial \theta}\right)\left(\frac{\partial L^*}{\partial \theta}\right)'\right)_{\theta=\bar{\theta}} .$$

$E(\bar{Q}_{\bar{\theta}})$ is the information matrix which indicates the amount of information from the data on the parameters which we are estimating. Also the inverse of the information matrix is the variance of the estimator. The proof is omitted since it involves detailed manipulation of the derivatives of the concentrated log-likelihood function, and the use of the identity for the information matrix (see, e.g., Kendall and Stuart (1961, Chapter 18) and Theil (1973, Section 8.4)).

Let

$$H = E(\bar{Q}_{\bar{\theta}})$$

and define

$$R = \sum_{t=1}^{T} (p_t - q_t)(p_t - q_t)'. \qquad (3.16)$$

Then $\text{plim}\, \frac{1}{T} R = \lim_{T\to\infty} E\left(\frac{1}{T}(p - q)(p - q)'\right)$,

thus R provides a consistent positive definite estimator of $-H$, which can be used in a quasi-Newton optimisation algorithm if and only if u_t is independently identically normally distributed.

The basic algorithm is:

$$\sum_{t=1}^{T} (p_t - q_t)(p_t - q_t)'\Delta\theta^{(r)} - \lambda^{(r)}(p - q) = 0$$

that is

$$\theta^{(r+1)} = \theta^{(r)} + \lambda^{(r)} \left[R^{-1}(p - q)\Big|_{\theta^{(r)}}\right]$$

$$= \theta^{(r)} + \lambda^{(r)} d^{(r)}, \qquad (3.17)$$

where $\lambda^{(r)}$ is chosen to $\max_{\lambda} L^*\left(\theta^{(r)} + \lambda d^{(r)}\left(\theta^{(r)}\right)\right)$ by a line search.

R must be positive definite, but there is a possibility that R may approach a singular matrix as the process iterates. Thus, we need to restrict R.

We let α be a prescribed positive constant less than one. Then at each iteration, we require

$$\rho = \frac{d'g}{d'd} > \alpha , \qquad 0 < \alpha < 1 \tag{3.18}$$

where $g = p - q$,

this will ensure the algorithm moving downhill. It ρ drops below α on a pariticular iteration, we whould replace R by a matrix with larger diagonal elements.

All gradient methods require a line search to determine the scalar λ after calculating the direction, d. Given that λ is chosen by such a line search algorithm (Section 2.4), together with the restriction on R, and given that $L^*(\theta)$ is twice continuously differentiable, we can now state the convergence theorem.

Consider the sequence

$$\theta^{(1)}, \theta^{(2)}, \ldots,$$

where

$$\theta^{(r+1)} = \theta^{(r)} + \lambda^{(r)} d^{(r)}$$

and

$$d^{(r)} = (R^{(r)})^{-1} g^{(r)} .$$

If $R^{(r)}$ obeys the restriction (3.18) and $\lambda^{(r)}$ is chosen to satisfy $L^*(\theta^{(r)} + \lambda^{(r)}d^{(r)}) > L^*(\theta^{(r)})$, then $\lim_{r\to\infty} g^{(r)} = 0$.

Not every critical point of $L^*(\theta)$ is a local maximum since saddle points can occur. If the iterative process chooses a value of θ where $L^*(\theta)$ has a saddle point, the iterative process will stall, as $g = 0$ at such points. However it is more likely that the process will find a local maximum which is not a global maximum. To safeguard against the possibility of accepting convergence to a local maximum that is not a global maximum, we choose several initial values of θ. If they do not all lead to convergence to the same point, then we might investigate the actual shape of the function with more care until the global maximum is located.

3.2 The BHHH Algorithm

The basic interation is:

Step 0: For each i, j, k and t; $i, j = 1, \ldots, n$; $k = 1, \ldots, K$; $t = 1, \ldots, T$

Compute: f_{it}, J_{ijt}

$$\underset{\sim}{S} = \left(\underset{\sim}{S}_{ij}\right) = \left[\sum_t \frac{f_{it}f_{jt}}{T}\right]$$

$$\underset{\sim}{S}^{-1} = \left(\underset{\sim}{S}^{ij}\right)$$

$$Y_{it} = \sum_j \underset{\sim}{S}^{ij} f_{jt}$$

$$H_{ijt} = (J_{ijt})^{-1}$$

Step 1:

Compute: $\frac{\partial f_i}{\partial \theta_k}$, $\frac{\partial J_{ij}}{\partial \theta_k}$ for each t

$$p_{kt} = \sum_{ij} H_{ijt} \left(\frac{\partial J_{ij}}{\partial \theta_k} \right)_t$$

$$q_{kt} = \sum_{i} \left(\frac{\partial f_{it}}{\partial \theta_k} \right) y_{it}$$

$$\mu_{kt} = p_{kt} - q_{kt}$$

Repeat Steps 0 and 1 for all t and k.

Step 2:

Compute: $$g = \sum_{t=1}^{T} \mu_{kt}, \qquad k = 1, \ldots, K ,$$

$$R_{ij} = \sum_{t=1}^{T} \mu_{it}\mu_{jt}, \quad i, j = 1, \ldots, n$$

Step 3: Compute new direction

$$d^{(r)} = (R_{ij})^{-1} g$$

Step 4: Check for convergence:

(i) $$\max_i \frac{|d_i^{(r)}|}{\max(1, |\theta^{(r)}|)} \leq \varepsilon_1$$

(ii) $\|g\|_2 \leq \varepsilon_2$

(iii) $\left| \dfrac{\theta_i^{(r)} - \theta_i^{(r-1)}}{\theta_i^{(r-1)}} \right| \leq \varepsilon_3$, for all i

(iv) $\left| \dfrac{L^*(\theta^{(r)}) - L^*(\theta^{(r-1)})}{L^*(\theta^{(r)})} \right| \leq \varepsilon_4$

If any of the conditions is statisfied, go to Step 6.

Step 5:

(a) Search for $\lambda^{(r)}$ using a line search procedure to ensure that

$$L^*(\theta^{(r)} + \lambda^{(r)} d^{(r)}) > L^*(\theta^{(r)})$$

(b) Update $\theta^{(r)}$ by setting

$$\theta^{(r+1)} = \theta^{(r)} + \lambda^{(r)} d^{(r)}$$

(c) Return to Step 0.

Step 6: If convergence is achieved, report parameter estimates $\hat{\theta}$ and its estimated variance-covariance matrix $(R_{ij})^{-1}$.

The BHHH algorithm is implemented in the computer programs described in Chapter 5.

CHAPTER 4

A METHOD OF SPECIFICATION, DIFFERENTIATION AND COMPUTATION FOR SETS OF GENERAL FUNCTIONS

4. A Differentiation Program

To estimate non-linear simultaneous equations systems by the method of maximum likelihood, it is necessary to compute the gradient of the log-likelihood function either analytically or by the use of numerical approximation. It was decided to implement the BHHH method and the Gill-Murray-Pitfield algorithm in our estimation program; both methods employ analytical gradient, hence a specific differentiation program is written for such purpose (Sargan and Chong (1980)).

4.1 Organisation of the Differentiation Program

The differentiation program may be divided into three parts:

1. To read in a specification of a set of functions and code it in a form easily translated and implemented in computer memory.

2. To differentiate such a set of functions, and to hold the specifications of the derivatives in computer memory.

3. To calculate the values of the functions and derivatives for given values of the variables.

The organisation of the differentiation program is shown in Figure 4.1.

The set of non-linear functions is first read into the computer memory in FORTRAN IV definitions. The definitions are then encoded into a list of integers representing the appropriate input symbols. A formula processor subroutine is called to process the list of integers into function specifications in a machine internal code and these are then stored permanently. When all input functions have been processed, differentiation can begin. Each of the components of function specifications are considered in turn and applied the appropriate differentiation rule. The resultant derivatives are defined as functions in the same internal code as function specifications. When all functions have been differentiated, an evaluation routine is called to decode the internal code and then compute the functions and derivatives values. The output from the differentiation program prints only the numerical values, not the functions in normal FORTRAN expressions.

4.2 General Considerations and Function Specifications

If we follow the usual FORTRAN conventions as to the definitions of a function with "*" and "/" having priority over "+" and "-", we will find our more complicated expressions having brackets whenever a factor in a product is the sum of a series of terms. Thus we will simplify our computing and differentiating by introducing a NEW function NFUNC corresponding to the contents of the brackets, whenever brackets are used in the definition of the function.

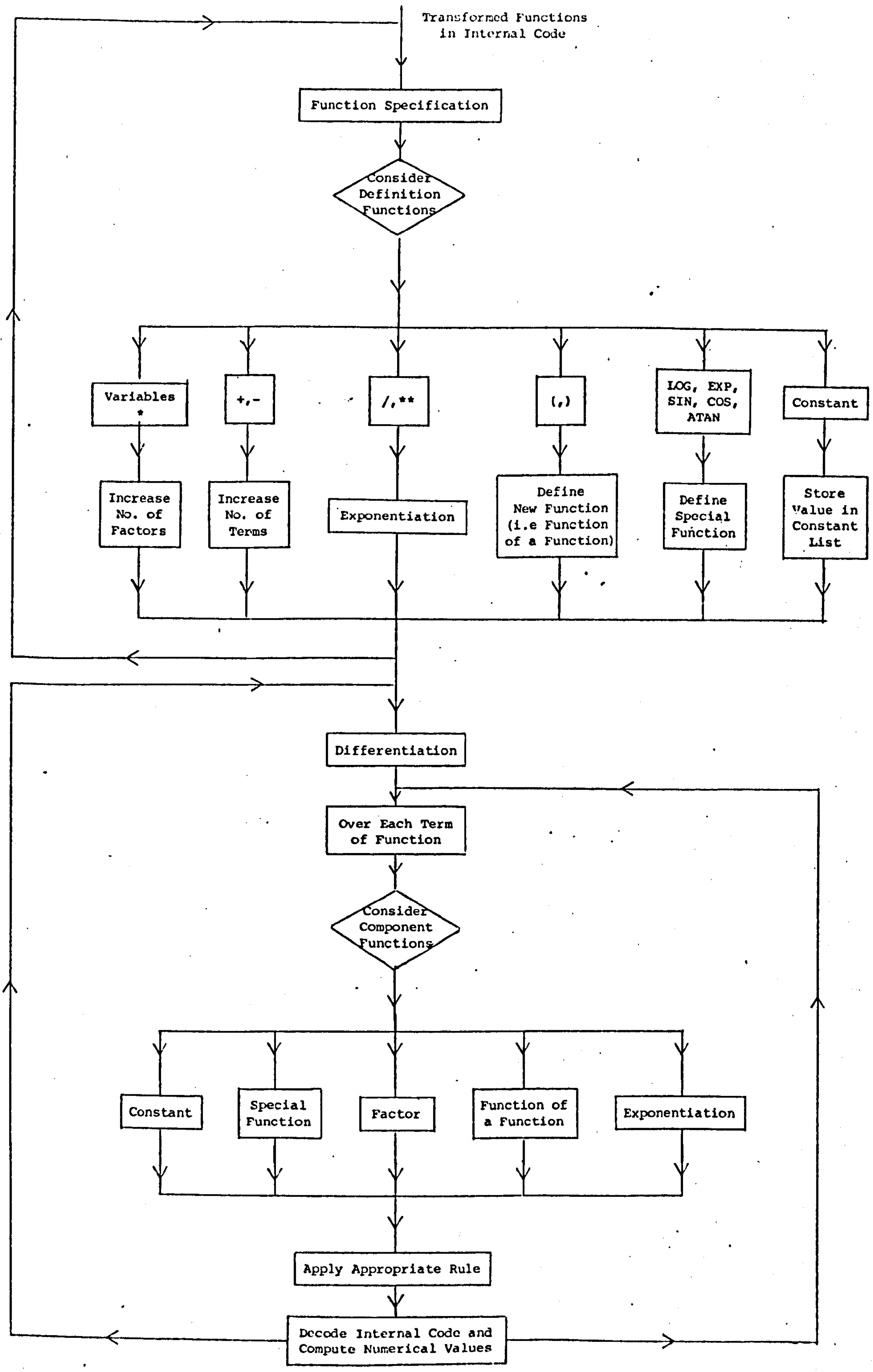

Transformed Functions in Internal Code
Function Specification
Consider Definition Functions
Variables *
+,-
/,**
(,)
LOG, EXP, SIN, COS, ATAN
Constant
Increase No. of Factors
Increase No. of Terms
Exponentiation
Define New Function (i.e Function of a Function)
Define Special Function
Store Value in Constant List
Differentiation
Over Each Term of Function
Consider Component Functions
Constant
Special Function
Factor
Function of a Function
Exponentiation
Apply Appropriate Rule
Decode Internal Code and Compute Numerical Values

Figure 4.1

In addition to "*", "/", "+", "-", we wish to introduce "**", "LOG", "EXP", "SIN", "COS" and "ATAN". These will be called SPECIAL FUNCTIONS and denoted by F_k.

We then define a set of "defined functions" as follows:

$$f_s = \sum_{i=1}^{I} c_i \prod_{j=1}^{J_i} \phi_{ij} \tag{4.1}$$

where the ϕ_{ij} are described as FACTORS and the products of the factors are defined as TERMS. (Of course, more correctly, every I, J_i, c_i, ϕ_{ij} should have a suffix s.)

The c_i are real constants, and should be chosen from a store or list of constants created as the definitions are read into memory.

The factors ϕ_{ij} are of three types:

(i) $\phi_{ij} = (x_k)^p$

where x_k is some variable in the set of variables;

(ii) $\phi_{ij} = (f_k)^p$

where f_k is some function previously defined;

(iii) $\phi_{ij} = (F_k(x_t))^p$ or $(F_k(f_t))^p$.

In all three cases, p is an exponent (which corresponds to a "**" in the original input).

The specifications of the functions are held as a set of integers, one after the other, so that space is not wasted. Also the definitions follow one another in the order in which the definitions are read in, not in the order in which they will need to be computed. To compute any function in the correct entry, it would be necessary to have an array of pointers for the order of computation. This array need only list the functions in priority of computations or perhaps contain the addresses of the start of each function specification.

Suppose we discriminate between indices relating to variables by saying that:

(a) integers $\leq$ 1000 refer to variables.

(b) integer $i > 1000$ that $i - 1000$ is the index of the corresponding function.

(c) However, each factor may be a special function, so we allocate the first five integers (1 to 5) to indicate special functions:

that is, LOG = 1
EXP = 2
SIN = 3
COS = 4
ATAN = 5

Note that we do not allow a special function of a special function unless this is done by using a defined function.

4.3 Sets of Conventions for Defining a Function

(i) Constant Indices

We have set up a set of conventions for constants as follows:

(a) An integer one means there is no constant for the current term or function, that is, $c_1 = 1.0$, for example, Exp x_1 becomes 1.0 * Exp x_1.

(b) Positive sign means plus, with an INDEX corresponding to the order in a vector of constant CONS. The value of the constant can be found in element (INDEX-1) of vector CONS. For example, value of c_5 can be found in CONS (5-1).

(c) Negative sign means minus with the constant held as (b) above.

(d) If the number of factors is zero, then the term only consists of a constant. This constant is defined in the same way as above.

(ii) Specifications of a Function

As we have suggested earlier, we use integers to represent a set of functional symbols. For all integers less than or equal to 1000, they represent variables and any integer $i > 1000$ then $i - 1000$ is the index of the corresponding function. We have allowed integers 1 to 5 to represent special functions such as LOG, EXP, SIN, COS and ATAN. Thus if $i \leq 1000$, we take $i - 5$ to be the index of a variable.

Now we suggest that the actual list of integers required for a given specification be as follows:

1. Number of function (i.e. defining order in list of functions).

2. Number of terms in function. In term of formula 4.1, this is I.

Then for each term we need to define:

(2a) Number of factors in the current term (which is J_i for each i).

(2b) Index of constant at the start of each term (i.e. index of c_i and the constants are stored in a list).

(2c) For each factor, an integer defining whether it is a variable, a special function, or a defined function.

(2d) For each special function a following index saying whether the function depends on a variable or a defined function.

(2e) A negative integer which occurs only if an exponent is used.

(iii) Function of a Function

A function can refer to another function with a separate definition provided that whenever this happens, we can arrange that the second function is computed earlier. There will be incorrect results if it is not possible to arrange a consistent order of computation.

(a) Functions with Bracket-Contents

We treat any bracket-contents of a function as a new function (NFUNC). When an open bracket is encountered on read in, a new function is immediately defined and the specification of this new function is stored in the definition list. The advantage of doing this is that it enables a function specification including brackets to be interpreted consecutively without providing temporary storage for bracket-contents definition, and has the advantage that in differentiation and numerical evaluation the contents of the bracket are differentiated or computed only once, rather than computed each time it occurs in the definition of the various order derivatives. A lower priority index is allocated to this new function in the order of computation, that is, a new function is placed in the front of the priority queue. We choose to use this convention so as to allow definitions of original functions to be non-consecutive (this corresponds to an unconditional jump in an ordinary program). We need to jump over the new function specification list and continue from there as we compute or differentiate the original function. As an example we have the sequence,

1010, -16, 477

which would mean function f_{10} then jumps to address 477 in the specification list and continues from address 477.

We use the integer -16 to mean this UNCONDITIONAL jump whenever a bracket-contents is defined as a new function and the following integer gives the address of the NEXT integer in the specification.

On reading in a specification, when brackets have been encountered, f_{10} would be the contents of the brackets, and in fact the specification f_{10} would immediately follow in the specification list. In implementation, it would be arranged that f_{10} was computed and differentiated first. The "unconditional jump" would be used, so that in then computing the original function the program could jump to the next factor or term.

We also note that the advantage of having the number of terms, and factors of each term specified, is that we can use a simple "DO" loop on implementation.

(b) Treatment of NFUNC

We need to have markers for the new functions that we defined as bracket-contents as we go along. But also the definitions are going to define a set of functions, which are numbered by the expression

"f_i = ..." where i = function number

as the start of the definition. Note also that we are going to define functions by taking derivatives. Suppose that we assume our largest model is written in the form

$$u_{it} = f_i(y_t, z_t, \theta) \qquad \begin{array}{l} i = 1, \ldots, n \\ t = 1, \ldots, T \end{array}$$

and the maximum value of n is 20, and y_t is an $1 \times n$ vector of endogenous variables (also of maximum dimension 20). Suppose also that in setting up the definitions of the f_i, we use n^* intermediate or defined functions f_i^* (bracket-contents), so that the total functions defined in this way is $n + n^*$. Suppose that $n^* \leq 20$. It is suggested that we should permanently store the definition of

$$\begin{array}{ll} f_i & i = 1, \ldots, n \\ f_i^* & i = 1, \ldots, n^* \end{array}$$

and also the definitions of

$$\frac{\partial f_i}{\partial y_j} \qquad \begin{array}{l} i = 1, \ldots, n \\ j = 1, \ldots, n \end{array}$$

$$\frac{\partial f_i^*}{\partial y_j} \qquad \begin{array}{l} i = 1, \ldots, n^* \\ j = 1, \ldots, n \end{array}$$

Now if we wish to compute its derivatives with respect to θ (suppose θ was of dimension $m \le 50$), we need to compute

$$\frac{\partial f_i}{\partial \theta_k}, \quad \frac{\partial f_i^*}{\partial \theta_k}$$

$$\frac{\partial^2 f_i}{\partial y_j \partial \theta_k}, \quad \frac{\partial^2 f_i^*}{\partial y_j \partial \theta_k} \qquad \begin{array}{l} i = 1, \ldots, n \\ j = 1, \ldots, n \\ k = 1, \ldots, m \end{array}$$

Thus at each iteration (of the optimisation program), we need to compute $(n+n^*)(n+1)(m+1)$ functions. On this basis, if we store all functional specifications, we would have up to $40 \times 21 \times 51 \approx 40{,}000$ specifications, and if we allow up to 20 indices per specification, this means that the specification list (NLIST) would require 800,000 words which seems to be very unreasonable. So it is suggested that we should modify this.

Suppose we store the specification of f_i, f_i^*, $\partial f_i/\partial y_j$, $\partial f_i^*/\partial y_j$ permanently, and then store $\partial f_i/\partial \theta_k$, $\partial f_i^*/\partial \theta_k$, $\partial^2 f_i/\partial y_j \partial \theta_k$, $\partial^2 f_i^*/\partial y_j \partial \theta_k$ only temporarily, so for each k, we work out the specifications of these derivatives, then compute their numerical values for all t. Then move on to $(k+1)$ writing the specifications for the derivatives with respect to θ_{k+1} over those for θ_k.

In this way it is only necessary to store the specifications for $2(n+n^*)(1+n)$ functions at the time, that is 1680 specifications (say up to 30,000 words). We might reduce this to 25,000 words on the grounds that not all n, n^* and the number of words per specification would take their maxima in any one model.

Now what this means directly for NFUNC is that we reserve the function values 1 to n (where n is the number of equations in the model) for the explicitly defined functions, and then start the implicitly defined functions (the bracket-contents) consecutively from $n+1$ to $2(n+n^*)(n+1)$. Each time we define a new function either as the contents of the bracket, or as a derivative of one existing function, we increase NFUNC by one. At the end of the differentiation w.r.t. y_t, NFUNC should have reached $n+n^* + n(n+n^*)$, and at the end of that round of differentiations we take note of the corresponding NFUNC, that is set MAXF = NFUNC. Then after differentiating w.r.t. θ_k and computing the resulting derivatives, we reset NFUNC = MAXF, the address for storing derivative specifications back to the address corresponding to function NFUNC, and we then write the new specifications over the old specifications.

(c) Priority Ordering

The most difficult aspect of this procedure is to ensure that functions are defined in an approriate order of computation. We choose the usual convention that the lower index function in a priority list is computed earlier. To compute the function and to obtain the form of derivative functions it is necessary to ensure that we order the computations so that the value of function "B" is computed before function "A" which depends on function "B". Thus if we have an index of computing priority, then we must ensure that function "B" has a lower index than function "A" if "A" depends on "B".

We find it convenient to keep two lists:

(i) NPRIOR (j) shows the order in which f_j is computed; NPRIOR (1) = j shows f_j is computed first, NPRIOR (2) = k shows that f_k is computed second and so on.

(ii) We also invert this ordering by also listing NPRS (j) which shows for each j, the number of the function which is j in the priority ordering.

Each time a function is defined, it is taken next in the priority ordering. Now each time the definition of a function i refers to function j, it is checked that j occurs first in the ordering by comparing NPRIOR (i) and NPRIOR (j). The test should be passed if j is always defined before i. But if there is a misorder then first j is checked, by considering the NPRIOR for each function occurring in its definition, so that NPRIOR (j) is set at the greatest of these plus one. Then NPRIOR (i) is set at NPRIOR (j) + 1. Note that in order to do this it will be necessary to increase the priorities attached to all functions with priorities between the earlier NPRIOR (i) and NPRIOR (j) by one, but these can be located easily by using NPRS. NPRS must then be reallocated by using NPRS (NPRIOR (i)) = i. This procedure of checking the order of functions should be repeated if any reordering has been done.

(iv) Exponent

To introduce "**" operation, we treat "/" as "**-1". It seems worthwhile from the computing point of view to treat separately the cases where the exponent is a small positive or negative integer from other exponents, and to ensure that we do not waste space by adding unnecessary indices to the specification list when generally no exponent is necessary. In particular we need x^2, x^3, x^4 etc.

to be in a form when the computer can easily recognise that, for example, $\frac{d^2}{dx^2}(x^3) = 6x$ with no exponent on the x, or $\frac{d}{dx}(x^2) = 2x$ and so on.

Thus it is suggested that the exponent be held immediately following the factor to which it refers as a negative number. Thus in computing the value of the function on differentiating, we test after each factor to see whether the next integer in the specification list is negative. If so we realise there is an exponent, and we can then interpret the index to get the exponent. Care must be taken here as we come to functions defined implicitly by brackets, we need to test whether this negative integer "belongs" to the inner function or the outer function by means of the address of the unconditional jump.

From the computing point of view, there is no point in distinguishing large integers, and it is suggested that we take p the exponent only if

(i) it is an integer

and

(ii) $-15 \leq p \leq 10$ this allows, for the fact that if we differentiate five times x^{-10}, we end up with x^{-15}.

It is suggested that if the integer in the specification is $-j$, and $j \leq 26$, then we take $p = j - 16$ as the exponent, but if $j > 26$, then we take $p = c_{(j-26)}$.

Note that in the case $j > 26$, we would be in fact computing

$$|x|^p$$

or

$$|f|^p$$

since we would use $\exp(p \log |x|)$.

An Example

Consider the following sequence of integers:

24, 3, 2, 5, 10, 1036, 3, -3, 1, 10, 6, 1010, 2, 1, 2, 6, 1005

Here

"24"	shows that this is f_{24} specification.
"3"	shows that it has three terms.
"2"	shows that the first term has two factors.
"5"	shows that it starts with constant c_4.
"10"	corresponds to x_5.
"1036"	corresponds to f_{36}.
"3"	shows that the second term has three factors.
"-3"	shows a minus sign at the start of the term, that is, the term is $-c_2 * (\cdot)(\cdot)$.
"1"	shows special function LOG.
"10"	corresponds to x_5.
"6"	corresponds to x_1.
"1010"	corresponds to f_{10}.
"2"	shows the third term has two factors.
"1"	shows that there is no constant for this term.
"2"	shows the special function EXP.
"6"	corresponds to x_1.
"1005"	corresponds to f_5.

Thus we can translate this sequence into

$$f_{24} = c_4 * x_5 * f_{36} - c_2 * \text{Log } x_5 * x_1 * f_{10} + \text{Exp } x_1 * f_5$$

For expressions having exponents, we consider the example below:

$$f_{20} = c_4 * x_7 * f_{10}/x_9 + c_6 * f_{11} ** 2 * x_1$$

which is translated as

20, 2, 3, 5, 12, 1010, 14, -15, 2, 7, 1011, -18, 6,

where -15 indicates a "**-1" that is "/" and -18 is an exponent of **2 (i.e. $p = -j - 16$). If

$$f_{10} = x_7 ** c_6,$$

then the sequence of integers would be

10, 1, 1, 1, 12, -32,

where -32 corresponds to $c_{(-j-26)}$.

Note that when the exponent is not an integer, we are in fact taking the modulus of the variable, function or defined function.

(v) Reading in a Specification

The difference between our computer specification and reading a general FORTRAN function is that we allowed no brackets (except for the brackets that are always used in connection with special functions). All that is needed is to read in a more complicated function with brackets to define a new function when brackets occur. Thus, as soon as opening brackets "(" occur on the read in, a new function NFUNC is defined, and a jump (-16) is inserted over the definition of this function.

As an example, we have

(a) $$f_{16} = c_{10} + c_{11} * (c_{12} + c_{13} * x_{10}^{2}) * \text{Exp} (c_{14} * f_{12})$$

Then this would be translated as

$$f_{16} = c_{10} + c_{11} * f_{105} * \text{Exp}\ f_{106}$$

with

$$f_{105} = c_{12} + c_{13} * x_{10} ** 2$$

$$f_{106} = c_{14} * f_{12}$$

or another example

(b) $$f_{16} = \text{Exp} (c_{17} + c_{18} * (c_{19} + f_{12}) ** 2)$$

then

$$f_{16} = \text{Exp}\ f_{21}$$

$$f_{21} = c_{17} + c_{18} * f_{22} ** 2$$

and

$$f_{22} = c_{19} + f_{12}$$

Note that when a bracket has been opened, when the close bracket ")" is reached it would be checked whether the name of a variable or function or special function following variable or function is all that is in the bracket, if so the bracket is ignored (unless two consecutive special functions would be created by removing the bracket).

Example (b) is the one where brackets are nested. There is no problem with this provided enough information is stored to resume after the bracket.

The most important information is the address of the jump address, so that when the close bracket ")" is reached, the address of the next instruction entry can be found and stored after the integer -16 in the specification list.

Thus in reading, we need an index say NDEPTH of the level of nested brackets:

NDEPTH = 0 meaning we have no brackets
= 1 we have a function arising from a bracket
= 2 we have a function arising from 2 nested brackets.
⋮

Then we need an array JUMPAD(I,J) for the jump address connected with brackets of depth J with function I.

The important points to be remembered are:

(a) the number of terms that have already been read in the functions outside the bracket;
(b) the number of factors that have already been read in the current term;
(c) whether the previous operator was "/" (meaning that it will be necessary to insert **-1 later as exponent).

Thus we need three temporary lists to keep the intermediate values of (a) - (c) generated on reading in the function.

As a function is read in, two indices are held: NTERM and NFACT to indicate the number of terms and number of factors respectively. NTERM starts as 1 and is increased by 1 after reading "+" or "-". NFACT is stored in the appropriate address of the specification list when "+" or "-" is read, it is then set to zero, and increased by one whenever "*" or "/" is read.

It is necessary to remember which function is being defined (outside the bracket). We use NFUNC as the number of functions currently being processed and increase NFUNC by one for each bracket J. Similarly we need to remember the address in the specification list of the number of factors in the current term, this is the address where NFACT will be stored at the next "+" or "-". Note that each time a closing bracket is found, NDEPTH is decreased by one, the definition of the function in the bracket is completed, and the definition of the lower level function is resumed.

(vi) Characters for Input

The following is a list of characters which can only be used to construct a set of equations:

List	1	2	3	4	5	6	7	8	9	10	11
Character	V	F	*	/	+	-	0	1	2	3	4

List	12	13	14	15	16	17	18	19	20	21	22
Character	5	6	7	8	9	.	)	=	L	E	S

List	23	24	25	26	27	28	29	30	31	32	33
Character	C	A	N	G	X	P	I	O	R	T	(

To input any equation, users may construct any functional form of the equation from these 33 characters.

Some Remarks

1. A variable is represented by the character V, for example, V_1, V_{10}.
2. Equation name is represented by F, for example,

   F1 is equation 1

   F2 is equation 2
3. Operators are +, -, *, /, **.
4. Digits are 0 to 9.
5. Decimal is "•".
6. Brackets are used to define intermediate functions, for example, $V_{10}/((V_1 * V_2 + V_3) * \text{Exp } V_6)$.
7. "=" enables an expression to be read more easily, for example, $F_2 = V_1 * V_2 + 1/2 * V_3$
8. Characters are

   L, E, S, C, A, N, G, X, P, I, O, R, T.

   These enable us to set up special functions such as LOG, EXP, SIN, COS, ATAN. Also these may be used to construct the key word "NEXT" for the continuation of an equation on a second card.

4.4 Differentiation

When differentiating it is assumed that we wish to store a similar specification for the derivative. This may not be necessary if we require the derivative to be calculated for various values of the variables. In this case it is assumed that the specification of an appropriate set of derivatives is stored temporarily in public storage, and a calculation subroutine then interprets these specifications to get the numerical values for given X (the data matrix).

In cases where it is necessary to calculate second or higher order derivatives, it will be necessary to be able to trace which specification gives the first derivative of which function w.r.t. which variable. Thus, we prepare a one-dimensional array NADR(I) which stores addresses at the start of function I and a two-dimensional array NDER(I,J) which stores the function NFUNC of the derivative of function I w.r.t. variable J.

Thus to find the address of $\partial^2 f_i/\partial x_j \partial x_k$ we would first locate NFUNC of $\partial f_i/\partial x_j$ in array NDER(I,J), then look up NFUNC of NDER(I,J) differentieated w.r.t. variable x_k, and the corresponding new NFUNC and its address will lead to the derivative function $\partial^2 f_i/\partial x_j \partial x_k$.

The specification of derivative is based on the formula:

$$\frac{\partial\phi}{\partial x_s} = \sum_i \sum_k C_i * \prod_{j \neq k} (F_j)^{p_j} * \frac{\partial F_k}{\partial f_a} * \frac{\partial f_a}{\partial x_s} * p_k F_k^{(p_k - 1)} \qquad (4.2)$$

for a function of the form:

$$\phi = \sum_i c_i \prod_j \left[F_k(f_a)\right]^{p_k}$$

Note that the total number of terms may be equal to the total number of factors. (It will be less whenever a variable occurs rather than a defined function.)

In the most general case, in each term of the derivative $(J_i - 1)$ of the factors are the same as $\Sigma(J_i - 1)$ factors of the corresponding term of the function. The simplest treatment is to copy the specification of the term until we reach factor k, and then insert the terms that correspond to the derivatives. We then copy the remaining factors in the original term. Note that if the factor does not contain a special function we can omit the factor $\partial F_k/\partial f_a$. If a special function is a function of a variable then we check whether this is the variable with respect to which we are differentiating. If not we omit this term from the derivative (by not increasing our running count of the number of terms in the derivatives and increase k by one immediately, that is, go on to the next value of k). If the variables are the same, then we omit this factor from the term, that is, set $\partial f_a/\partial x_s = 1$. Finally if there is no exponent, then we can omit the last factor of equation (4.2) from the derivative function.

$\partial f_a/\partial x_s$ is a defined function, $\partial F_k/\partial f_a$ is another special function of f, except in two cases:

(i) for log f, we insert $^1/f$, that is, we have a factor f followed by the exponent "**-1".;

(ii) for ATAN f (i.e. $\tan^{-1}$ f), we need to insert $^1/(1+f^2)$. The way to do this is to define a new function $1+f^2$, while ensuring that $1+f^2$ is computed before the derivative function.

As each term in the derivative function is generated, the computer must remember the address where the number of factors is stored. Then as it looks at each factor it keeps a count of the number of factors so that at the end of the specification of that term it can insert the number of factors into the right palce in the specification list. Similarly it keeps a running count of the number of terms in the derivatives, which at the end of generating the total specification can be inserted into the second place in the specification list of that function. Notice that using these rules a term which is linear in a variable, may end up with a constant, and there is no need to take special heed, provided that we agree that a constant can occur as a term in any order in a function.

4.5 Simplification

Ultimately it must be stressed that it is worthwhile simplifying the functions and derivatives to avoid repetitive calculation.

(i) Eliminating Surplus Functions

As a new function is defined either on reaching outside specifications or by differentiation, the definitions of the existing function are scanned, and if an existing function is found to have exactly the same definition, then the new function is cancelled.

(ii) Cancelling Repeated Factors in Differentiating

In differentiating a special function factor such as EXP, LOG, SIN, COS, or ATAN; in each case there is the possibility that one of the other factors in this term is the same as the derivative of this factor. So each time we differentiate a factor of this type, we run through all the other factors in the term and if they are the same as the derivative factor, we increase the exponent of this factor by one.

(iii) Replacement of Simple Functions

The basic idea is that in the case where the derivative of a function is a single term, and where that function is used as a factor in defining a second function (as the contents of a bracket), then in differentiating the second function, we replace the derivative of the factor by its definition as a product of factors.

4.6 Numerical Evaluation of Function and Derivative Values

To evaluate function values, we need to compute all functions with lower indices in the priority list first. Intermediate functions such as bracket-contents and derivative functions generated by the process of differentiation can be picked up easily from the specification lists as the indices of the head address of all function specifications are stored in an array of pointers.

To calculate the function and derivative values for a set of given values, X, the computer interprets each function specification as a mathematical expression and then evaluates the function value. All function specifications must have their priorities checked before any function evaluation to get the right order of computation.

Intermediate function values are held in a temporary list pointed by the function number NFUNC. When an original function depends on the intermediate function NFUNC, it only needs to compute the original function value, then pick up the numerical value of NFUNC from temporary storage and then update the original function value with the value of NFUNC. Hence it does not have to recompute the same NFUNC value whenever any function refers to it.

4.7 Example

Consider the following example with two equations

(a) $(\log (x_1 + x_2 * x_3)) ** 2 = f_1$

(b) $x_1 + x_2 * \log (x_1 + x_3) = f_2$

If we call equation (a) f_1 and equation (b) f_2, then on reading in the first equation, the program will translate equation (a) as follows:

$f_1 = f_{100} ** 2$ (we take 100 as an arbitrary number)

$f_{100} = \log f_{101}$

$f_{101} = x_1 + x_2 * x_3$

where f_{100} is the outer bracket-contents and f_{101} is the inner bracket-contents. f_{100} and f_{101} are defined as intermediate functions.

Since f_1 depends on f_{100} and f_{100} depends on f_{101}, the priority ordering of function f_1 in the priority list would be:

index	
1	101
2	100
3	1
⋮	⋮

Where f_{101} has a lower index than f_{100} and f_1. Therefore we need to compute f_{101}, then f_{100} and finally f_1 in this ordering.

For the treatment of a new function number NFUNC, whenever a new function such as bracket-contents is defined implicitly, we increase the value of NFUNC by one. Also derivative functions are considered as new functions and hence NFUNC would have to be increased by one each time when a new function is generated by the differentiation.

In equation (a)

NFUNC = 100 means $\log f_{101}$

NFUNC = 101 means $x_1 + x_2 * x_3$

Note that if there is only one structural equation in this example, then NFUNC = 102 would be the derivative function differentiated w.r.t. any of the variables. Since we have two structural equations here, we need to let the following consecutive NFUNC value denote the bracket-contents of the second equation unless all the following structural equations are independent (i.e., non-nested) functions.

For example, in equation (b), we have

$$f_2 = x_1 + x_2 * \log f_{102}$$

$$f_{102} = x_1 + x_3 .$$

Now f_{102} has a lower index in priority list than f_2 which means f_{102} must be computed or differentiated before f_2.

The priority list for f_1 and f_2 would be

index	
1	101
2	100
3	1
4	102
5	2
⋮	⋮

that is, NPRIOR (1) = 101

NPRIOR (2) = 100

NPRIOR (3) = 1

NPRIOR (4) = 102

NPRIOR (5) = 2

and the reverse ordering of all functions would be

```
NPRS  (101)  =  1
NPRS  (100)  =  2
NPRS  (1)    =  3
NPRS  (102)  =  4
NPRS  (2)    =  5
```

that is, function 101 is the first function to be differentiated and computed, then function 100 and so on.

Now for the derivative function NFUNC (from 103 onwards) would be increased by one each time when a new derivative function is generated, therefore each value of NFUNC would represent an equation for the derivative function.

To compute function values, we have to pick up NFUNC from the priority list to get the correct order of function to be computed. But to compute the derivative values, we compute each derivative function NFUNC by setting

```
NFUNC  =  NDER (I,J)
```

where NDER is a two-dimensional array to store the derivative of function I differentiated w.r.t. variable J . Again NFUNC must have its priority checked before any numerical evaluation.

CHAPTER 5

A COMPUTER PROGRAM FOR THE ESTIMATION OF GENERAL NON-LINEAR ECONOMETRIC MODELS

5. An Estimation Program

In this chapter, we describe a computer program called NLMLE (Non-Linear Maximum Likelihood Estimation) which estimates a small to medium size non-linear econometric model by the method of maximum likelihood.

The numerical techniques applied to the program are:

(i) The BHHH method.

(ii) The variable-metric method of Gill-Murray-Pitfield.

Both methods employ analytical derivatives for the computation of the gradient of the concentrated log-likelihood function.

Generally, non-linear econometric models are either non-linear in parameters, variables or both. When non-linear in the variables y_t, that is, when J_t (where $J_t = \partial f_t/\partial y_t'$) varies over t, there will be substantial computation to calculate $\partial f_t/\partial y_t'$.

NLMLE is designed to tackle this kind of highly non-linear model with complex econometric functions. It enables users to define the set of simultaneous equations in functional form. The equations are input to the computer together with the attached data, the choice of optimisation technique and line search procedure, a tolerance level for the accuracy of the estimates and a maximum number of iterations for the model to run.

The output from the program comprises the computed parameter estimates, their standard errors and the T-ratios, the residual sum of **squares** matrix and the asymptotic variance-covariance matrix of the parameter estimates.

5.1 Organisation of the Estimation Program

The estimation program is divided into three major parts:

(i) The differentiation program.

(ii) The optimisation procedures and line search.

(iii) Some supporting routines for a convergence test, the initialisation of a new step-size for each iteration and for calculation of output statistics.

Figure 5.1 illustrates **the** flow of the estimation program.

After input, the differentiation program is loaded to differentiate the set of equations. The analytic gradient and Hessian matrix are then set up. (The Hessian matrix depends on the choice of the optimisation procedure.) The optimisation method then maximises the likelihood function of the set of equations.

If convergence has been achieved, the procedure terminates and the supporting routines will print out relevant statistics. If convergence has not been achieved, then the program updates the current value of parameter estimates with the new step-size calculated from a line search procedure. It then repeats the process until it has satisfied the convergence criterion or it has reached the maximum number of iterations.

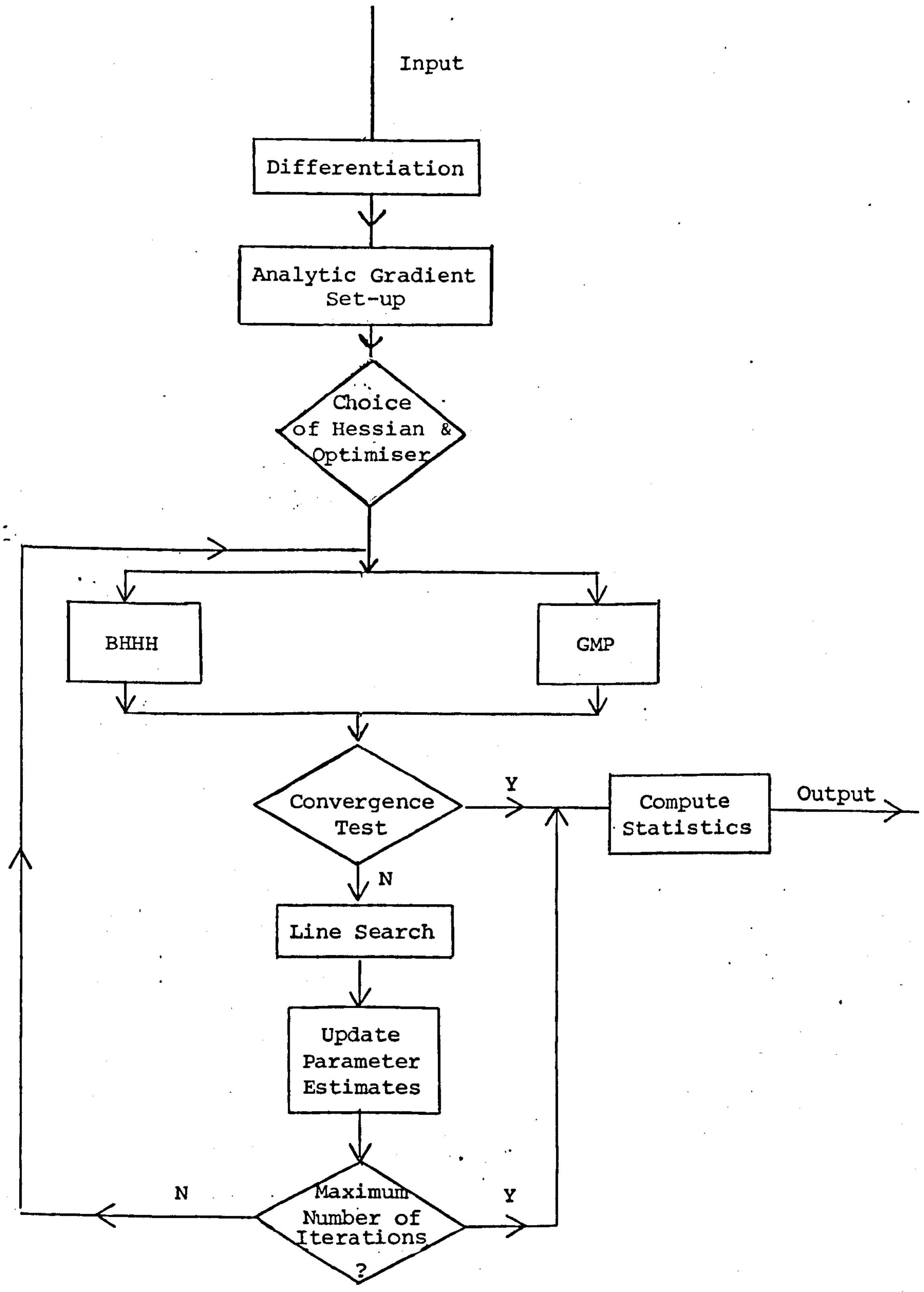

Input
Differentiation
Analytic Gradient Set-up
Choice of Hessian & Optimiser
BHHH
GMP
Convergence Test
Y
N
Compute Statistics
Output
Line Search
Update Parameter Estimates
Maximum Number of Iterations ?
N
Y

Figure 5.1

5.2 Functional Definitions

We define the set of equations according to the function specifications described in Chapter 4. It is important that all equations must be specified according to the conventions set up in the previous chapter.

Usually, users need not be concerned with the internal workings of the differentiation program, but some knowledge of the representation of expressions and the way they are defined should be acquired in order to use NLMLE more easily, efficiently, and effectively.

We differentiate the set of equations in the following steps:

(i) differentiate with respect to the endogenous variables y_t to get the Jacobian, that is $\partial f_t/\partial y_t'$;

(ii) differentiate with respect to the parameter θ_k, that is $\partial f_t/\partial \theta_k'$;

(iii) differentiate the Jacobian with respect to parameter θ_k, that is $\partial^2 f_t/\partial \theta_k \partial y_t'$.

Repeat (ii) and (iii) for all k, $k = 1, \ldots, K$.

Following the functions being differentiated, an evaluation routine is called to evaluate the numerical values of the derivative functions. When the evaluator sees a factor, it checks to see whether the factor has a value assigned to it, if there is a value, it updates the function value. If it sees a function as an argument, again it checks the function and updates the current function value. If there is a special function attached to the factor or function, it applies the special function to the evaluated argument. If it is division or exponentiation, the same treatment is applied as with the special function.

The evaluator scans each function term by term and factor by factor. It returns the final value of each function.

A packing routine is then loaded to pick up all the derivative values and put them in a compact form as the gradient of the concentrated log-likelihood function, that is,

$$g = \frac{\partial \operatorname{Log} L^*(\theta)}{\partial \theta} = \sum_i \sum_j \sum_t \left(J_{ijt}\right)^{-1} \left(\frac{\partial J_{i,j,t}}{\partial \theta}\right) -$$

$$\frac{T}{2} \sum_t \left(\frac{\partial f_t}{\partial \theta}\right)' \left(\sum_t \frac{f_{it} f_{jt}}{T}\right)^{-1} f_t \qquad (5.1)$$

where (J_t), $\left(\frac{\partial J_{i,j,t}}{\partial \theta}\right)$ and $\left(\sum_t \frac{f_{it} f_{jt}}{T}\right)$ are all $n \times n$ matrices.

5.3 Estimation Methods

A gradient method and a variable metric method by Gill-Murray-Pitfield are provided. The two methods offer different choices for the Hessian matrix. The first (METHOD = BHHH) is that described in Chapter 3. The second method offered (METHOD = GMP with analytical derivatives) differs from the first only in the calculation of the Hessian matrix. For this method, the updating rule is described in Chapter 2.

The BHHH routine is specially programmed and implemented in NLMLE. For GMP, NLMLE uses a routine from the NAG library for the optimization.

5.4 Program Composition

The program is written in FORTRAN IV and was developed on both CDC 7600 and ICL 2980 computers. The DAP versions applying parallel processing will be described in Chapter 6.

The two serial versions comprise a main section and 18 subroutines.

FIMLX	the main section.
INPUT	reads in data decks and sets up any lags required.
DATALT	allows a variety of data transformations to be performed.
RDCARD	reads in equations.
FRML	formula processor to process the input equations into machine internal code.
NUMBER	reads in constants, variable and function indices and exponentiation of the input equations.
DIFF	differentiates equations.
BHHH	Brendt-Hall-Hall-Hausman estimation procedure.
DIFIML	sets up equations for differentiation.
DIEVAL	packing routine for derivative functions.
EVAL	evaluation routines for original and derivative functions.
GCHECK	gradient check routine using finite differences.

FUNML	routine to calculate log-likelihood function.
GSTEP	line search.
BARD	line search by BARD.
INVERT	matrix inversion routine using Gauss-Jordan full pivoting.
PRIOR	checks priority ordering of function.
PQEVAL	evaluation of gradient.

Input to NLMLE

$$\text{IMETH} = \begin{cases} 0 & \text{method = BHHH} \\ 1 & \text{method = GMP (analytic derivatives)} \\ 2 & \text{method = GMP (finite differences)} \end{cases}$$

$$\text{ISTEP} = \begin{cases} 0 & \text{linear search = GSTEP} \\ 1 & \text{linear search = BARD} \end{cases}$$

IMAX	maximum number of iterations.
X	data matrix.
N	the number of parameters θ.
V	a $1 \times n$ array containing an estimate of the position of the best available initial value $L^*(\theta)$.
TOLB	tolerance level for the termination criterion.
NSQZ	number of iterations in linear search.
NB	number of stochastic equations in the system.
NINTF	number of intermediate functions.
NVAR	number of variables (y_t and z_t).
NT	number of observations.
NL	number of lags
NI	number of identities
NY	number of endogenous variables (y_t)
NZ	number of predetermined variables (z_t)

The overall input is terminated by four dollar signs, that is, $$$$.

A user's guide to NLMLE is given in Appendix C.

Output of NLMLE

(a) At each iteration, option to print:

(i) old and new function values, new step-size and number of function calls for that iteration;

(ii) gradient and gradient norm; weighted-gradient, i.e. $g'H^{-1}g$;

(iii) direction vector $\underline{d}^{(i)}$;

(iv) parameter estimates $\underline{\theta}^{(i)}$;

(b) At the end of the iterative procedure, information regarding:

(i) whether the program converged and the number of iterations used;

(ii) maximum number of function calls;

(iii) the log-likelihood function value;

(iv) the final parameter estimates;

(v) the estimated asymptotic variance-covariance matrix of the parameters $\hat{\theta}$;

(vi) the standard errors and T-ratios;

(vii) the residual sum of squares **matrix**.

Limitations

The following apply to the CDC 7600 version of the program:

(i) A maximum of 20 equations.

(ii) A maximum of 30 parameters.

(iii) A maximum of 100 observations.

(iv) A maximum of 50 variables.

The version on the ICL 2980 can estimate a larger model of up to 100 parameters and $>> 100$ observations.

The three parallel DAP versions are restricted to five-equation models with a maximum of 20 parameters and 30 variables but up to 4096 observations.

The program listing is given in Appendix **B**, and an example of the output in Appendix **D**.

CHAPTER 6

NON-LINEAR ECONOMETRIC MODELLING ON A PARALLEL PROCESSOR

6.1 Potential Role of the Distributed Array Processor for Research in Economics

The ICL Distributed Array Processor (DAP) is a 64×64 array of micro-processors embedded in the store of a host computer, each processor being associated with 4K bits of semi-conductor store (which can be accessed by the host if the DAP is not in use). Clearly, taking the procesor to the data (rather than vice-versa) avoids the time usually required to route information.

Conventional computers use sequential operating procedures and upper limits exist for the speed of calculation possible using such an approach. Miniaturisation and micro-circuits are part of an effort to resolve such problems.

However, a DAP presents a radically different potential solution, using parallel computation; moreover, while the DAP is operating, the host is free to carry out other tasks. Thus to add two 64×64 matrices on a 64×64 DAP takes the same time as adding two scalars and any task which can be tackled in 64 parallel streams on a 64 cell array takes 64^{-1} of the time for 64 sequential operations.

Users of the DAP will have to learn new ways of conceptualising their objectives. The main idea can be seen by considering the multiplication of two $N \times N$ matrices A and B. In conventional FORTRAN the algorithm would be a programmed version of:

$$C = AB \Rightarrow C_{ij} = \sum_{k=1}^{N} a_{ik} b_{kj}$$

which can be rewritten as the inner product

$$C_{ij} = \underline{a}'_{\cdot i} \underline{b}_{j\cdot}$$

where $A' = (\underline{a}_{\cdot 1}, \ldots, \underline{a}_{\cdot N})$, $B = (\underline{b}_{1\cdot}, \ldots, \underline{b}_{N\cdot})$.

In the DAP, parallel computation would exploit the outer product from:

$$C = \sum_{k=1}^{N} \underline{a}_{k\cdot} \underline{b}'_{\cdot k}$$

Each micro-processor does N multiplications in sequence and cumulates the total. Similar reformulations apply to matrix inversion, etc.

Research in Economics is invariably multivariate and hence is intensive in the use of matrix operations. For example, econometric estimation usually entails maximising a scalar function of matrices, with prolific use of inversion and multiplication of large dimensional matrices. Similarly, recent advances in computing economic equilibria require massive array calculations which consume a considerable amount of cpu time. Monte-Carlo simulation is intensively used by econometricians both to study the properties of econometric estimators and to model the behaviour of economic systems with a large number of participants. Finally, investigating the finite sample distributions of procedures for system estimation does create major demands for time on available computer systems.

Large-scale econometric models are generally non-linear in both the variables used in estimation and the parameters of the likelihood function. Few systems of this kind have been appropriately estimated because the computational time required is very large. With the introduction of array processors that are capable of executing a large number of instructions simultaneously, the computational time can be substantially reduced.

In order to estimate the system of equations, $L^*(\theta)$ (3.11) has to be maximised with respect to θ, which is a formidable task for large values of n and k, where n is the number of equations in the system and k is the number of parameters. Also if T is large, it is equally difficult to compute $\sum_{t=1}^{T} \log (\text{abs}|J_t|)$ due to the excessive amount of cpu time needed.

Many special cases of equation (3.11) have been investigated, and efficient methods for optimising the relevant likelihood function have been extensively programmed, for example, Hendry (1976), Hendry and Srba (1980), Hendry and Tremayne (1976). Many of the numerical optimisation methods are strongly oriented towards implementation on serial computers.

However, the Distributed Array Processor presents the possibility of a different solution. The power of the DAP is based on its high degree of parallel operation; hence a specially designed algorithm is essential so that the DAP can be fully exploited.

6.2 The Distributed Array Processor (DAP)

The basic concept of a parallel processor which can execute the same instruction on many data items has been known for many years. There have been several processors of this type built, most notably, STARAN and ILLIAC IV (Thurber and Wald (1975)). Although the DAP is similar in concept to these machines, it has two important differences:

(i) the number of processing elements (PEs): the DAP has 4096 as opposed to 256 and 64 for the STARAN and ILLIAC IV, respectively;

(ii) the simplicity of the processing elements (PEs): the PEs in the DAP are one bit processors which means that all operations other than bit manipulations are done in software.

6.3 Architecture

The DAP is a 64×64 two-dimensional grid of PEs each with 4096 bits of local memory (the fact that there are 4096 PEs and 4096 bits of local memory is only coincidence). Each PE can perform two basic operations: one bit addition and one bit broadcast of data to one of its four neighbouring PEs (Gostick 1979, 1981; Parkinson 1976 (Nov.), 1977 (Nov.), 1980).

For the purpose of computation, we can describe the DAP as consisting of:

(i) 4096 store planes containing 64×64 bits.

(ii) The activity plane (A plane) of 64×64 bits. The setting of a particular bit in the A plane to 1 (that is, .TRUE.) allows the corresponding PE to perform a given instruction; that is, the A plane acts as a 'MASK' as to whether an instruction is executed in a particular PE or not.

(iii) A 64×64 array of PEs that are each connected to their four nearest neighbours.

6.4 Programming the DAP

The DAP has two programming languages: APAL and DAPFORTRAN. APAL is a low level assembly language (ICL (1979)). DAPFORTRAN is an extension of standard FORTRAN. The DAP will execute all standard FORTRAN statements except for formatted READ/WRITE commands (ICL (1981)). The additional facilities of DAPFORTRAN are basically two extra variable modes: vector and matrix together with a generalised indexing syntax to allow efficient use to be made of them. The three modes can be declared as follows:

```
INTEGER SCALAR_INTEGER, SCALAR_INTEGER_ARRAY(100)
INTEGER_VECTOR( ), SET_OF_INTEGER_VECTORS(,10)
INTEGER_MATRIX(,), SET_OF_INTEGER_MATRICES(,,15)
```

Note that ICL FORTRAN has always regarded the limitation of the length of variable names to 6 characters as being unnecessarily restrictive, and permits up to 32 characters for all names in a program. DAPFORTRAN follows this convention, thus permitting a much more sensible naming of variables, routines, etc., and hence giving more readable programs. Since spaces are not permitted within DAPFORTRAN names, it is desirable to have some alternative method for breaking up long names. For this purpose the underscore character _ may be used (as in 2900 system Control Language). This character is ignored by the compiler.

By the declaration VECTOR( ) we mean a vector with 64 components and, by MATRIX(,), a matrix of 64×64 components. Also sets of vectors and matrices can be declared as shown above. Similar declarations can be made for REAL, LOGICAL and CHARACTER variables.

All the normal arithmetic and logical operations are defined element by element for vector and matrix modes. For example, if A, B and C are REAL matrices, then

```
      A  =  B + C
```

means that A is the element by element sum of B and C. In standard serial FORTRAN the above statement is:

```
           DO  10  I = 1, 64
           DO  10  J = 1, 64
      10   A(I,J)  =  B(I,J) + C(I,J)
```

Moreover, arithmetic and logical operations can be performed on variables of different modes if there is no ambiguity. For example, if A and B are real matrices and C is a REAL scalar, then

```
      A  =  B * C
```

means that A is the element by element product of the matrix B and a matrix consisting of 4096 components all with the same value C.

The other significant feature of DAPFORTRAN is masked (or logical) assignment; that is, the assignment of one matrix to another can be 'masked' with a LOGICAL matrix. For example, if A and B are INTEGER matrices and MASK is the LOGICAL matrix defined by

```
MASK = A .GT. B
```

(i.e. an element of MASK is .TRUE. when the corresponding element of A is greater than the corresponding element of B).

Then

```
A(MASK) = B
```

means that the element by element assignment only takes place when the corresponding element of MASK is .TRUE.

The equivalent FORTRAN code for this statement is

```
      DO 10 I = 1, 64
      DO 10 J = 1, 64
      IF (A(I,J).GT.B(I,J))A(I,J) = B(I,J)
   10 CONTINUE
```

which is very inefficient on a serial processor whereas there is no difference in efficiency between A = B and A(MASK) = B on the DAP.

6.5 Examples

Clearly DAPFORTRAN is an ideal programming language when considering 64*64 matrices or matrices that can be partitioned into 64*64 submatrices. This does not mean that it is inflexible and cannot be used on problems of different dimensions; for example, we consider the problem of multiplying two N*N matrices A and B where $N \leq 64$. The following method is used:

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{11} \\ a_{21} & a_{21} \end{pmatrix} * \begin{pmatrix} b_{11} & b_{12} \\ b_{11} & b_{12} \end{pmatrix} + \begin{pmatrix} a_{12} & a_{12} \\ a_{22} & a_{22} \end{pmatrix} * \begin{pmatrix} b_{21} & b_{22} \\ b_{21} & b_{22} \end{pmatrix}$$

$$= \begin{pmatrix} a_{11}\ b_{11} & a_{11}\ b_{12} \\ a_{21}\ b_{11} & a_{21}\ b_{12} \end{pmatrix} + \begin{pmatrix} a_{12}\ b_{21} & a_{12}\ b_{22} \\ a_{22}\ b_{21} & a_{22}\ b_{22} \end{pmatrix}$$

$$= \begin{pmatrix} a_{11}\ b_{11} + a_{12}\ b_{21} & a_{11}\ b_{12} + a_{12}\ b_{22} \\ a_{21}\ b_{11} + a_{22}\ b_{22} & a_{21}\ b_{12} + a_{22}\ b_{22} \end{pmatrix}$$

(the operations * and + are element by element multiplication and addition, respectively).

The DAPFORTRAN code is:

```
      SUBROUTINE MATRIX_MULTIPLY (C,A,B,N)
C
C     This is a subroutine to multiply two N × N matrices  A  and  B
C     where  N ∈ {1, ..., 64}  and place the result in  C.
C     We assume that the contents of  A  and  B  are undefined
C     except for the N × N submatrix of values in the top left corner
C     of  A  and  B.
C
      REAL A(,), B(,), C(,)
      LOGICAL MASK(,)
      MASK = ROWS (N+1, 64) .OR. COLS (N+1, 64)
C
C     ROWS (N+1, 64)  is a LOGICAL MATRIX FUNCTION that creates a
```

```
C     LOGICAL matrix which has its first  N  rows set to .FALSE.  and
C     the remaining rows set to .TRUE. .COLS (N+1, 64)  has the same
C     definition, mutatis mutandis, with respect to columns.
C
      C = 0.0
      A (MASK) = 0.0
      B (MASK) = 0.0
      DO 10 K = 1, N
   10 C = C + MATC (A(,K)) * MATR (B(K,))
C
C     MATC (REAL_VECTOR)  is a REAL MATRIX FUNCTION that creates a
C     REAL matrix all of whose columns are equal to REAL_VECTOR.
C     MATR (REAL_VECTOR)  has the same definition, mutatis mutandis, with
C     respect to rows.
C
      RETURN
      END
```

A second example is the calculation of $C_i = A_i * B_i$, $i = 1, \ldots, 4096$, where A_i, B_i and C_i are all 5×5 (say) matrices. The appropriate segment of DAPFORTRAN code is:

```
      REAL A(,, 5,5),  B(,, 5,5),  C(,, 5,5)
      DO 10 I = 1, 5
      DO 10 J = 1, 5
      C(,,I,J) = 0.0
      DO 10 K = 1, 5
   10 C(,,I,J) = C(,,I,J) + A(,,I,K) * B(,,K,J)
```

This is identical to the equivalent code for a serial processor, except that, in every reference to a vector or array, the first subscript is preceded by two commas to indicate that the procedure is to be carried out in every processor simultaneously.

The corresponding FORTRAN code would be:

```
      REAL A(4096,5,5), B(4096,5,5), C(4096,5,5)
      DO 10 L = 1, 4096
      DO 20 I = 1, 5
      DO 20 J = 1, 5
      C(L,I,J) = 0.0
      DO 20 K = 1, 5
   20 C(L,I,J) = C(L,I,J) + A(L,I,K) * B(L,K,J)
   10 CONTINUE
```

6.6 Estimation Procedure and Implementation

The BHHH method is of a form suitable for parallel computation (see Chapter 3).

Three versions of the program were implemented:

(A) A parallel version on the DAP for models of up to 4096 observations.

(B) A parallel version on the DAP for between 65 and 128 observations.

(C) A parallel version on the DAP for models of up to 64 observations.

In the serial version (NLMLE, Chapter 5), we evaluate all the functions and derivatives at $\theta^{(i)}$ for each of the observations. Clearly, this is not the most efficient method. In version (A), the architecture of the DAP allows us to evaluate the functions of up to 4096 observations simultaneously.

In versions (B) and (C), we evaluate simultaneously $L^*(\theta^{(i)} + \lambda_\alpha d^{(i)})$ for 32 or 64 values of λ_α, respectively. This is because we are able to 'partition' the DAP into 32 or 64 'parallel processors' according to the number of observations. This allows us to find the optimal value of $L^*(\theta^{(i)} + \lambda_\alpha d^{(i)})$ in our test models with a grid search procedure in only one step.

To evaluate the log-likelihood function requires the following calculations:

(a) $\sum_{t=1}^{T} f_{it}f_{jt}$, for $i,j = 1, \ldots, n$

(b) $(J_t)^{-1}$, for $t = 1, \ldots, T$

(c) $\sum_{t=1}^{T} \log|\det J_t|$

On the DAP these calculations are performed very efficiently. The inner products (a) can be evaluated for a given i and j in two steps: firstly, we calculate $f_{it}f_{jt}$, $t = 1, \ldots, T$ simultaenously and, secondly, we find the summation in one operation.

The DAPFORTRAN code is:

```
      REAL F(,,N), INNER_PRODUCTS (N,N)
C
      DO 10 I = 1, N
      DO 10 J = 1, N
   10 INNER_PRODUCTS (I,J) = SUM (F(,,I) * F(,,J))
```

(SUM is an in-built DAPFORTRAN function that computes $\sum_{i}\sum_{j} A_{ij}$ for a 64×64 matrix (A_{ij})).

Similarly for (b), the inversion of up to 4096 $n * n$ matrices J_t can be performed in parallel on the DAP using Gaussian elimination and column pivoting. At the same time we obtain the determinant of J_t.

The DAPFORTRAN code for the inversion routine is shown in Appendix H.

Lastly, (c) can be written as one line of DAPFORTRAN

```
      REAL DET_JT(,), SUM_LOG_DETJT
C
      SUM_LOG_DETJT = SUM (LOG(DET_JT))
```

Versions (B) and (C) are similar to the above except that a separate summation in (a) and (c) is required for each λ_α. For example, the DAPFORTRAN code for (a) is:

```
      REAL F(,,N), INNER_PRODUCTS (N,N,L)
      LOGICAL ALPHA_MASKS (,,L)
C
C          L IS THE NUMBER OF GRID POINTS ON THE LINE
      DO 10 I = 1, N
      DO 10 J = 1, N
      DO 10 K = 1, L
   10 INNER_PRODUCTS (I,J,K) = SUM (MERGE (F(,,I) * F(,,J), 0.0,
     +ALPHA_MASKS (,,K)))
```

(MERGE (REAL_MATRIX_A, REAL_MATRIX_B, LOGICAL_MATRIX_MASK) is an in-built DAPFORTRAN function that produces a REAL matrix whose elements are the same as REAL_MATRIX_A if the corresponding element of LOGICAL_MATRIX_MASK is .TRUE., and equal to the corresponding element of REAL_MATRIX_B otherwise.)

In versions (B) and (C), we can now determine the optimum λ_α by evaluating $L^*(\theta^{(i)} + \lambda_\alpha d^{(i)})$ for all λ_α simultaneously.

To compute the gradient $\partial L^*/\partial\theta$ consists essentially of matrix multiplication and taking the trace of a matrix. The DAP can do both of these operations very efficiently. Finally we evaluate the Hessian matrix which is again a matrix product.

We have chosen a set of test models (Model (iii), Chapter 7) for our DAP programs. The timings and results are described in section 7.7.

CHAPTER 7

A SET OF NON-LINEAR MODELS

7. Non-linear Models Simulation

To test the NLMLE estimation program, we need to define sets of models which are simple to specify and graded by:

(i) size of the model with respect to the number of equations, n; variables, m; unknown parameters, k; and observations, T.

(ii) non-linearity (i.e. high, little, none) with respect to the unknown parameters, variables/or both

(iii) properties of data (i.e. inter-correlation)

(iv) white noise (i.e. random errors).

It is of great difficulty to obtain a realistic model with the above representation and structure because model building on such a system takes a long time to construct and collect the data. Thus we have decided to derive our non-linear system by Monte-Carlo simulation. An example of such typical non-linear model is a cross-section production model with large sample size, large parameter set, high non-linearity in the variables, moderate correlation of the data set and automatically white noise if we are sampling the data from a distribution.

It was decided to only generate the data of the model approximately to the true data by a Data Generation Process and then applied a Newton-type iterative solution to the system. We can vary the number of parameters by using the same model, but prespecify some of the parameters at fixed values to reduce the number of parameters requiring estimation.

Notice that by sampling a population $X_1,\ldots,X_T$ with the sample parameter $\bar{\theta}$, the error of $\bar{\theta}$ and its estimate $\hat{\theta}$ is of order $T^{-\frac{1}{2}}$, i.e.

we have the distribution of the sample population

$$D(X_1,\ldots,X_T|\bar{\theta}),$$

and if we apply the maximum likelihood estimation to the sample values

$$\max_{\theta} L\ (\theta|x_1,\ldots,x_T) = \hat{\theta}$$

then $(\hat{\theta} - \bar{\theta}) = O_p\left(\frac{1}{\sqrt{T}}\right)$,

where

O_p is the order in probability.

Hence when T is small, the error could be very large, but as long as the estimator is consistent, we would expect $\hat{\theta}$ converge asymptotically to the true value of the sample $\bar{\theta}$.

7.1 Modelling Considerations

Suppose we take $n = 2$ and $n = 5$ as the two different non-linear simultaneous systems, and that we use a combination of linear functions and arctangent to introduce variable non-linearity with respect to the endogenous variables. Notice that arctangent has the advantage that it is increasing for all values of X, and combined with a linear term is not likely to introduce multiple solutions. It would be appropriate to construct the model so that the function is a quadratic in the parameters and the variables raised to the power.

7.2 Model Specification

It was decided to specify:

for the $n = 2$ system:

$$\Omega_u = \sigma^2 \begin{bmatrix} 1.0 & 0.5 \\ 0.5 & 1.0 \end{bmatrix}$$

and for the $n = 5$ system:

$$\Omega_u = \sigma^2 \begin{bmatrix} 1.0 & 0.5 & 0.0 & 0.0 & 0.5 \\ 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\ 0.0 & -0.5 & 1.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.5 & 1.0 & -0.5 \\ 0.5 & 0.0 & 0.0 & -0.5 & 1.0 \end{bmatrix}$$

The model was chosen to be of a manageable size and generality. It was appropriate that the model be fully non-linear in the variables, and particularly that the Jacobians in each time period should be functions of both variables and parameters. It was decided to select the variables, so that the equations of the model could be easily solved for y_t as a function of u_t (so yielding the path of y_t for given u_t) by a Newton iterative solution method, starting from the path y_{ot} defined as the path corresponding to $u_t = 0$, or such that

$$f(y_{ot}, z_t, \theta) = 0.$$

Since the z_t are determined once and for all, and are fixed in repeated simulations, and since it is usual for there to be at least as many variables z_t as equations in the model (i.e. $m > n$), it was decided to introduce a set of z_{it}, such that z_{it} occurs only in $f_i(y_{ot}, z_t, \theta) = 0$, $i = 1, \ldots, n$. It was then possible to first determine y_{oit}, $i = 1, \ldots, n$, and z_{it}, $i = n+1, \ldots, m$, using any simple procedure, and then to solve the above equation to obtain z_{it}, $i = 1, \ldots, n$. This provides an initial solution path y_{ot}, which serves as the starting value for a Newton iteration to solve the more general equations. The model is of the form:

$$u_{it} = f_{it}(y_t, z_t, \theta), \quad \begin{array}{l} i = 1, \ldots, n \\ t = 1, \ldots, T \end{array}$$

We define some intermediate functions,

$$f^*_i(y_t) = \gamma_i \tan^{-1}(\alpha_i y_{it}) + \sum_j B_{ij} y_{jt} \tag{7.1}$$

In (7.1), all or most of the coefficients can be fixed a priori, for example, we could take $\gamma_i = 0.1$ and $B_{ij} = 0$ except $B_{ii} = 1$. A better alternative, which introduces a further non-linearity in $f_{it}(y_t, z_t, \theta)$ as a function of θ, is to write

$$B_{ij} = B_{oij} + B_{1ij}\theta_k + B_{2ij}\theta_k^2 \tag{7.2}$$

where the model contains only one or two parameters θ_k, and each B_{ij} is written as a quadratic in θ_1, or θ_2, with B_{oij}, B_{1ij} and B_{2ij} fixed a priori.

Now we write

$$u_{it} = (\eta_{ii} z_{it} + (z^2_{(k_i)t})^{\delta_i}) + f^*_i(y_t), \quad \begin{matrix} i = 1, \ldots, n \\ t = 1, \ldots, T \end{matrix} \tag{7.3}$$

where k_i depends on i, so that each equation contains two exogenous variables. For example, when $n = 2$, we take $k_1 = 3$ and $k_2 = 4$.

We generate the data with negligible error by using a Newton-type iterative solution method to solve the equations for a random u_{it}, starting the iteration from values of y_{jt} that correspond to $u_{it} = 0$. If $\eta_{ii} \neq 0$, we can set the y_{it} at some values y_{oit} and calculate $g^*_{it} = f^*_i(y_{ot})$ and $u_{it} = 0$, and then set $z_{(k_i)t}$ at some equally arbitrary values, and then solve

$$z_{it} = -\frac{1}{\eta_{ii}} \{(z^2_{(k_i)t})^{\delta_i} + g^*_{it}\} . \tag{7.4}$$

At this stage the y_{oit} are the solutions of the equations (7.3) when $u_{it} = 0$, for all i and t. We can compute z_{it} once and for all for a given model.

To generate N replications for a given model, we solve equation (7.3) only approximately. We generate u_{it} as jointly normal, and then add this into

$$y^*_{it} = -(\eta_{ii} z_{it} + (z^2_{(k_i)t})^{\delta_i}). \tag{7.5}$$

Now we write $y^{(r)}_t$ for the r th iterate with

$$y^{(o)}_t = y_{ot}$$

and

$$\Delta y_t^{(r)} = y_t^{(r)} - y_t^{(r-1)}$$

Then we use a Newton-type iteration for the solution of

$$f_i^* (y_t^{(r)}) = 0$$

and $y_t^{(r)} = y_t^{(r-1)} - f_i^* (y_t^{(r-1)})/f_i^{*\prime}(y_t^{(r-1)})$,

$$\left(\frac{\partial f_i^*}{\partial y_t}\right)_{y_t=y_t^{(r-1)}} \Delta y_t^{(r)} = \left(y_{it}^* - f_i^*(y_t^{(r-1)})\right) + u_{it} \qquad (7.6)$$

where u_{it} and y_{it}^* are computed with $r = 0$. We repeat the iteration, until $\|y_t^{(r)} - y_t^{(r-1)}\|$ is sufficiently small.

7.3 Data Generation Process

In order to consider a set of different models we take a basic model for $n = 2$ and $n = 5$ and then vary one parameter at a time.

Suppose we generate each $z_{(k_i)t}$ for $k_i > n$ independently (once for all) using the following equation:

$$z_{k_i t} - \lambda_k z_{k_i(t-1)} = \mu_k + U_{kt} \qquad (7.7)$$

where the U_{kt} are independently distributed as $\sim N(0, 1)$.

For the $n = 2$ case, we take only one k, and set $k_1 = 3$, $\lambda_3 = 0.5$, $\mu_k = 1.0$.

For the $n = 5$ case, we take $k_1 = 6$ and $k_2 = 7$, and set $\lambda_6 = 0.5$, $\lambda_7 = 0.7$, $\mu_6 = \mu_7 = 1.0$.

We then generate the values of y_{oit} using the same **form of equations** (7.7) by using y instead of z.

Now for $n = 2$, we generate:

y_{o1t} using $\lambda = 0.5$, $\mu = 2.0$;

y_{o2t} using $\lambda = 0.7$, $\mu = 2.0$.

In addition when $n = 5$, we generate:

y_{o3t} using $\lambda = 0.5$, $\mu = -1.0$;

y_{o4t} using $\lambda = 0.7$, $\mu = -1.0$;

y_{o5t} using $\lambda = 0.5$, $\mu = 0.0$.

Now for the values of B_{ij} in equation (7.2), we take $B_{oij} = 0$ for all models.

For $n = 2$, we take one parameter $\theta_k = \theta$, and set

$$\left(B_{1ij}\right) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\left(B_{2ij}\right) = \varepsilon * \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

where $\varepsilon = 0.5$.

For $n = 5$, we set

$$\left(B_{1ij}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(B_{2ij}) = \varepsilon * \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

where $\varepsilon = 0.1$, and we also set $\alpha_i = 1$ for all i.

Postulation

For the two systems and for all i, we fix the values of the parameters to be:

$\eta_{ii} = 5$

$\delta_i = 1$

$\gamma_i = 0.3$

$\alpha_i = 1$

$\theta_i = 1$.

We also fix $\sigma^2 = 0.5$ and $T = 20$.

With these quantities, we can proceed the Data Generation Process according to the specification of our models.

7.4 Sets of Models

It is proposed to generate one set of data for $n = 5$ models, and consider three values for the number of parameters p.

$n = 5$

(i) $p = 18$

We assume $\alpha_i = \alpha$ is one unknown, that B_{ij}, $i = 1, 2, 3$ depends on th unknown θ_1, and B_{ij}, $i = 4, 5$ depends on the unknown θ_2, and take γ_i, η_{ii}, δ_i all unknown for $i = 1, \ldots, 5$. This gives a total of 18 unknown parameters.

Now the model becomes:

$$f_1^*(y_t) = \gamma_1 \tan^{-1}(\alpha y_{1t}) + \theta_1 y_{1t} + 0.1 * \theta_1^2 y_{2t}$$

$$f_2^*(y_t) = \gamma_2 \tan^{-1}(\alpha y_{2t}) + 0.1 * \theta_1^2 y_{1t} + \theta_1 y_{2t}$$

$$f_3^*(y_t) = \gamma_3 \tan^{-1}(\alpha y_{3t}) - 0.1 * \theta_1^2 y_{2t} + (\theta_1 + 0.1 * \theta_1^2) y_{3t}$$

$$f_4^*(y_t) = \gamma_4 \tan^{-1}(\alpha y_{4t}) + 0.1 * \theta_1^2 y_{3t} + (\theta_2 - 0.1 * \theta_2^2) y_{4t}$$

$$f_5^*(y_t) = \gamma_5 \tan^{-1}(\alpha y_{5t}) + 0.1 * \theta_1^2 y_{2t} + 0.1 * \theta_2^2 y_{4t} + \theta_2 y_{5t}$$

and

$$u_{1t} = (\eta_{11} z_{1t} + (z_{6t}^2)^{\delta_1}) + f_1^*(y_t)$$

$$u_{2t} = (\eta_{22} z_{2t} + (z_{6t}^2)^{\delta_2}) + f_2^*(y_t)$$

$$u_{3t} = (\eta_{33} z_{3t} + (z_{7t}^2)^{\delta_3}) + f_3^*(y_t)$$

$$u_{4t} = (\eta_{44} z_{4t} + (z_{7t}^2)^{\delta_4}) + f_4^*(y_t)$$

$$u_{5t} = (\eta_{55} z_{5t} + (z_{7t}^2)^{\delta_5}) + f_5^*(y_t)$$

The unknown parameters are

γ_i, η_{ii}, δ_i, $i = 1, \ldots, 5$; one α; one θ_1 and one θ_2.

with 5 endogenous variables $y_{1t}, \ldots, y_{5t}$ and 7 exogenous variables $z_{1t}, \ldots, z_{7t}$.

(ii) <u>$p = 12$</u>

We assume the same model as in (i) but set $\theta_1 = \theta_2$ and $\delta_i = 1$. This reduces the number of parameters by 6, that is, we have γ_i, η_{ii}, $i = 1, \ldots, 5$, one α and one θ.

The model is in Appendix F.

(iii) <u>$p = 6$</u>

In addition to (ii), assume $\gamma_i = \gamma$ for all i and $\eta_{11} = \eta_{33} = \eta_{55} = \eta$, this reduces the number of parameters by another 6, that is, we have γ, α, θ, η, η_{22} and η_{44}.

The model is shown in Appendix F.

Thus from the set of generated data, we get three different optimisation problems.

<u>$n = 2$</u>

(iv) <u>$p = 9$</u>

Assuming only one θ, we have a maximum of 9 parameters, that is, 2 each of α_i, γ_i, η_{ii}, δ_i and one θ.

Thus we have the following model:

$$f_1^*(y_t) = \gamma_1 \tan^{-1}(\alpha_1 y_{1t}) + (\theta + \theta^2)y_{1t} + \theta^2 y_{2t}$$

$$f_2^*(y_t) = \gamma_2 \tan^{-1}(\alpha_2 y_{2t}) - \theta^2 y_{1t} + (\theta + \theta^2)y_{2t}$$

and

$$u_{1t} = (\eta_{11}z_{1t} + (z_{3t}^2)^{\delta_1}) + f_1^*(y_t)$$

$$u_{2t} = (\eta_{22}z_{2t} + (z_{3t}^2)^{\delta_2}) + f_2^*(y_t)$$

(v) <u>$p = 6$</u>

We constrain $\alpha_i = \alpha$, $\gamma_i = \gamma$, $\delta_i = \delta$, and so leave 6 parameters, that is, α, γ, δ, η_{11}, η_{22} and θ.

The model is shown in Appendix F.

(vi) <u>$p = 4$</u>

Finally, in addition to (v), if we take $\eta_{ii} = \eta$ and $\delta = 1$, we get a 4-parameter model, that is, γ, α, θ and η.

Again the model is shown in Appendix F.

If we take the 6-parameter model (for $n = 2$) as standard, we can then vary the level of the parameters one at a time from their correct values.

7.5 <u>Alternative Values of Parameters</u>

We considered the following alternative values for the sets of non-linear models:

(i) $T = 50$

(ii) $\sigma^2 = 0.1$

(iii) $\gamma_i = 0.5$

(iv) $\varepsilon = 1.0$

(v) $\delta_i = 0.7$

Each of these values has a describable general tendency:

(i) increased sample size;

(ii) reduced error variance;

(iii) reduced non-linearity of f as a function of endogenous variables;

(iv) increased non-linearity with respect to parameters affecting the determination of the endogenous variables;

(v) reduced non-linearity with respect to exogenous variables' parameters.

We start by generating data for standard $n = 2$ model with $T = 50$, where the first 20 observations give us the sample for $T = 20$. We then take this data for $T = 20$, and the standard 6-parameter model and try NPOINT = 10 starting points. The first are all the parameters at their correct values, and the remainder are chosen so that for any parameter, for example,

$$\gamma = \bar{\gamma}(1 + h),$$

where h is chosen at random from the interval $(-0.5, +0.5)$. After we have seen what computing time is requird for this experiment, we can then decide whether to use NPOINT = 10 for the other models.

Note that we have:

3 models of $n = 5$ with different values of p.

3 models of $n = 2$ with different values of p.

5 non-standard models of $n = 2$ with $p = 6$.

Using 10 starting points for all models, yields a total of 11 models × 10 = 110 models.

Note that for each run, not only is a new starting point chosen but new values of u_{it} are generated. But we can calculate z_{it} once and for all, and then for a given model calculate g^*_{it}, and keep these values unchanged for different runs. The actual y_t used can be retained constant, and the same data used for models differing only by p.

7.6 Estimation Results and Computer Timings

We present some numerical results for particular runs of models (i) to (vi) estimated by the methods of BHHH and GMP with analytical derivatives. GMP (with numerical approximation to the derivatives) was used in various models and model (iii). Since there were only six unknown parameters in model (iii) it was worth trying this method for the $n = 5$ system because the number of function evaluations to approximate the gradient was relatively smaller than for models (i) and (ii). Model (iii) was also used to test the DAP program and the results from the DAP runs will be discussed in section 7.7.

Since the run time for each model starting with the true values was rather long, we were unable to test all the models with 10 different starting points except for model (v) where we varied the parameter γ (Table 11). However, for other models, we estimated with the true starting values and also shifted 0.05 unit away from the true values except for model (i), in this case we only shifted 0.025 unit away. Also σ^2 was chosen to be small (although previously we suggested $\sigma^2 = 0.5$) so that the models might converge more quickly. To test the sensitivity of the methods to σ^2, we tested models (iv) to (vi) by varying σ^2 from 0.1 to 0.5, and the results of these runs are shown in Tables 4-6. Tables 10a and 10b show the efficiency of the methods when T is small.

We now present the results from models (i) to (iii), with $n = 5$, $T = 50$, $\sigma^2 = 0.01$, $\varepsilon = 0.1$, $\gamma_i = 0.3$, $\alpha = 1.0$ and $\delta_i = 1.0$.

(a-i) <u>Model (i), p = 18</u>

Initial values = True values of parameters

<u>Table 1a Final Estimates of Parameters</u>

Parameters	Initial Values	BHHH(1) (Old Line Search)	BHHH(2) (Modified Line Search)	GMP (Analytical Derivatives)
γ_1	0.3	0.3035	0.3035	0.3045
γ_2	0.3	0.3410	0.3410	0.3410
γ_3	0.3	0.3081	0.3081	0.3080
γ_4	0.3	0.3031	0.3031	0.3032
γ_5	0.3	0.2993	0.2993	0.2993
α	1.0	0.9725	0.9725	0.9726
θ_1	1.0	1.0001	1.0001	1.0001
θ_2	1.0	0.9992	0.9992	0.9992
η_{11}	5.0	5.0132	5.0132	5.0133
η_{22}	5.0	5.0287	5.0287	5.0288
η_{33}	5.0	5.0012	5.0012	5.0012
η_{44}	5.0	5.0020	5.0020	5.0020
η_{55}	5.0	4.9994	4.9994	4.9994
δ_1	1.0	1.0021	1.0021	1.0021
δ_2	1.0	1.0023	1.0023	1.0023
δ_3	1.0	1.0001	1.0001	1.0001
δ_4	1.0	1.0001	1.0001	1.0001
δ_5	1.0	0.9990	0.9990	0.9990

Table 1b Details of Iterative Convergence

Method	No. of Iterations	No. of † Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) seconds
BHHH(1)	58	108	-940.897488	-950.924755	434.6
BHHH(2)	38	61	-940.897488	-950.924748	229.0
GMP	25	68	-940.897488	-950.924769	601.9

Note:

(1) Old line search where the initial step-size is fixed to one.

(2) Modified line search where the initial step-size is adjusted using algorithm 2.4.1 of Chapter 2.

† Number of function calls is the total number of function evaluations in the iterative procedure.

The log-likelihood function values are set to 6 decimal places due to the flatness of L*.

(a-ii) Model (i), p = 18

Initial values = Shifted true values of parameters

Table 1c Final Estimates of Parameters

Parameters	Shifted Initial Values	BHHH[1] (Old Line Search)	BHHH[2] (Modified Line Search)	GMP (Analytical Derivatives)
γ_1	0.275	0.3035	0.3035	0.3035
γ_2	0.275	0.3410	0.3410	0.3410
γ_3	0.275	0.3081	0.3081	0.3080
γ_4	0.275	0.3031	0.3031	0.3031
γ_5	0.275	0.2993	0.2993	0.2993
α	0.975	0.9726	0.9725	0.9725
θ_1	0.975	1.0001	1.0001	1.0001
θ_2	0.975	0.9992	0.9992	0.9992
η_{11}	4.975	5.0132	5.0132	5.0133
η_{22}	4.975	5.0287	5.0287	5.0288
η_{33}	4.975	5.0012	5.0012	5.0012
η_{44}	4.975	5.0020	5.0020	5.0020
η_{55}	4.975	4.9994	4.9994	4.9994
δ_1	0.975	1.0021	1.0021	1.0021
δ_2	0.975	1.0023	1.0023	1.0023
δ_3	0.975	1.0001	1.0001	1.0001
δ_4	0.975	1.0001	1.0001	1.0001
δ_5	0.975	0.9999	0.9999	0.9999

Table 1d Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) seconds
BHHH(1)	111	235	-447.747959	-950.924767	877.1
BHHH(2)	96	186	-447.747957	-950.924762	703.7
GMP	57	108	-447.747957	-950.924769	861.1

Note:

Model (a-i) was also estimated with the initial values shifted 0.05 unit away from the true values. None of the above methods converged to the final estimates of the parameters. It was realised that the model was badly identified with the γ's. So a set of linear restrictions was introduced, that is, by setting

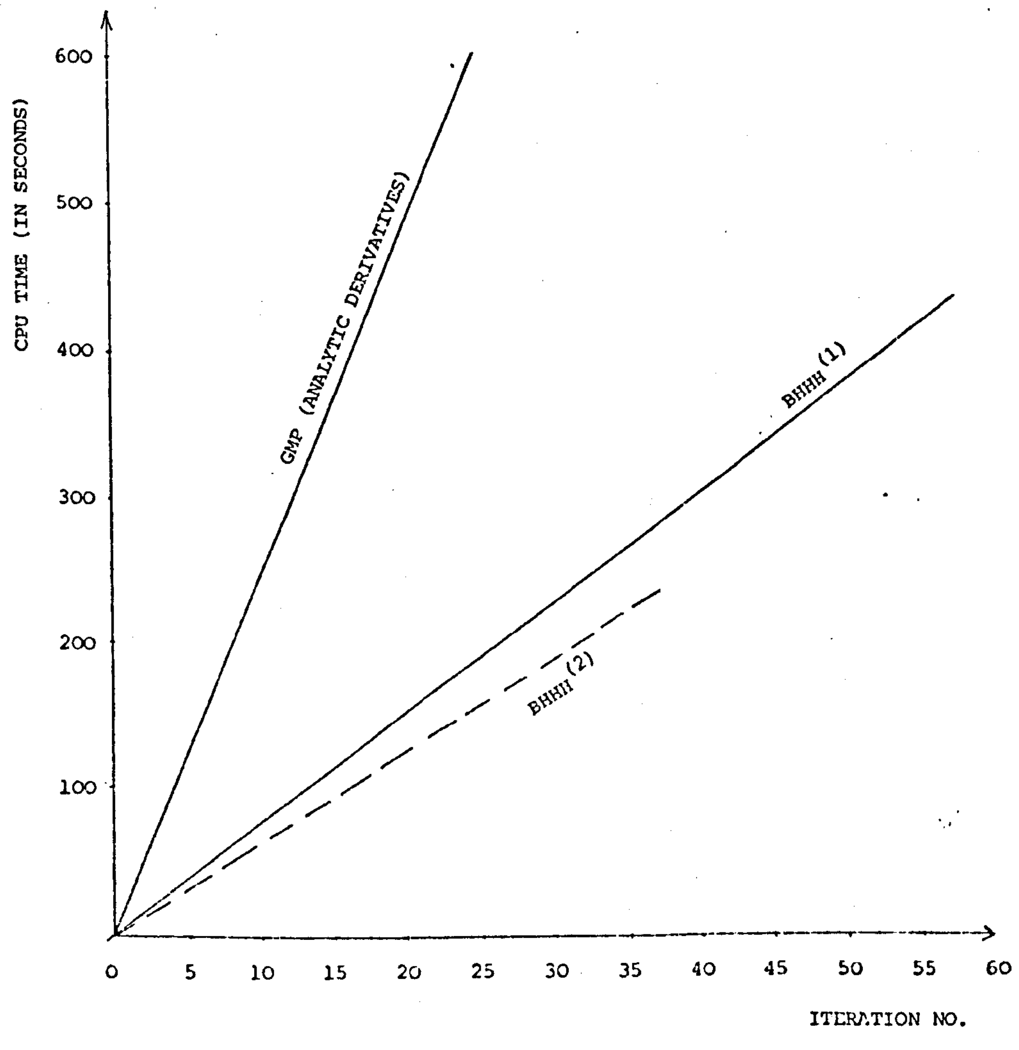
$$\gamma_4 = 0.6 - \gamma_3$$

and

$$\gamma_5 = \gamma_1 + \gamma_2 - \gamma_3$$

and the model was re-estimated wtih its true values and the shifted values (0.05 away). From these two runs, both the GMP and BHHH failed to converge after a substantial amount of CPU times (800 seconds and 1200 seconds respectively). The GMP method failed to achieve convergence for this model with starting values of parameters shifted away by 0.05 because the initial setting of the function value was unreliable. And for the BHHH, because the starting values were badly approximated to the final estimates, the method would not converge at all.

To ensure that model (a-i) converged to the same optimum points apart from starting from the true values, we decided to re-shift the parameters 0.025 unit away from the true values and estimated the model again. The results from these runs are shown in Tables 1c and 1d.



NOTE: SLOPE SHOWS TIME PER ITERATION.

Figure 7.1

Tables 1 (a and b) illustrate the estimated parameters and CPU times for model (i). The BHHH procedure with the modified line search seems to be a more efficient method in terms of CPU time. It is faster than the GMP (with analytical derivatives) by a factor of 2½ and converged to the same set of optimum values.

The modified line search has reduced the number of iterations and function evaluations substantially (Table 1b), in this respect, the CPU time was reduced by half (BHHH$^{(2)}$) due to the more accurate line search during the iterative procedure.

Figure 7.1 shows the iteration numbers against the CPU times for the three estimation procedures for model (a-i) to achieve convergence. Clearly BHHH$^{(2)}$ is the most satisfactory optimisation technique for this application.

GMP (with numerical approximation to the derivatives) method was also used but the model failed to converge after a substantial amount of CPU time (1200 seconds). This procedure is not recommended for such models unless the analytical derivatives of the likelihood function cannot be obtained easily.

(b-i) Model (ii), p = 12

Initial values = True values of parameters

Table 2a Final Estimates of Parameters

Parameters	Initial Values	BHHH[(1)] (Old Line Search)	BHHH[(2)] (Modified Line Search)	GMP (Analytical Derivatives)
γ_1	0.3	0.2914	0.2914	0.2913
γ_2	0.3	0.3201	0.3201	0.3201
γ_3	0.3	0.3189	0.3189	0.3189
γ_4	0.3	0.3066	0.3066	0.3066
γ_5	0.3	0.3058	0.3058	0.3058
α	1.0	0.9592	0.9592	0.9593
θ	1.0	0.9975	0.9975	0.9975
η_{11}	5.0	4.9884	4.9884	4.9884
η_{22}	5.0	4.9996	4.9996	4.9996
η_{33}	5.0	4.9999	4.9999	4.9999
η_{44}	5.0	5.0002	5.0002	5.0002
η_{55}	5.0	5.0009	5.0009	5.0009

Table 2b Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) seconds
BHHH[(1)]	17	25	-940.897488	-948.419153	59.8
BHHH[(2)]	18	26	-940.897488	-948.419157	63.0
GMP	19	45	-940.897488	-948.419164	249.4

(b-ii) Model (ii), $p = 12$

Initial vlaues = Shifted true values of parameters

Table 2c Final Estimates of Parameters

Parameters	Shifted Initial Values	BHHH[(1)] (Old Line Search)	BHHH[(2)] (Modified Line Search)	GMP (Analytical Derivatives)
γ_1	0.25	0.2913	0.2913	0.2913
γ_2	0.25	0.3201	0.3201	0.3201
γ_3	0.25	0.3189	0.3189	0.3189
γ_4	0.25	0.3066	0.3066	0.3066
γ_5	0.25	0.3058	0.3058	0.3058
α	0.95	0.9593	0.9593	0.9593
θ	0.95	4.9975	4.9975	4.9975
η_{11}	4.95	4.9884	4.9884	4.9884
η_{22}	4.95	4.9996	4.9996	4.9996
η_{33}	4.95	4.9999	4.9999	4.9999
η_{44}	4.95	5.0002	5.0002	5.0002
η_{55}	4.95	5.0009	5.0009	5.0009

Table 2d Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) seconds
BHHH[(1)]	46	233	-524.748891	-948.419160	553.8
BHHH[(2)]	36	105	-524.748891	-948.419161	253.3
GMP	41	84	-524.748891	-948.419164	430.4

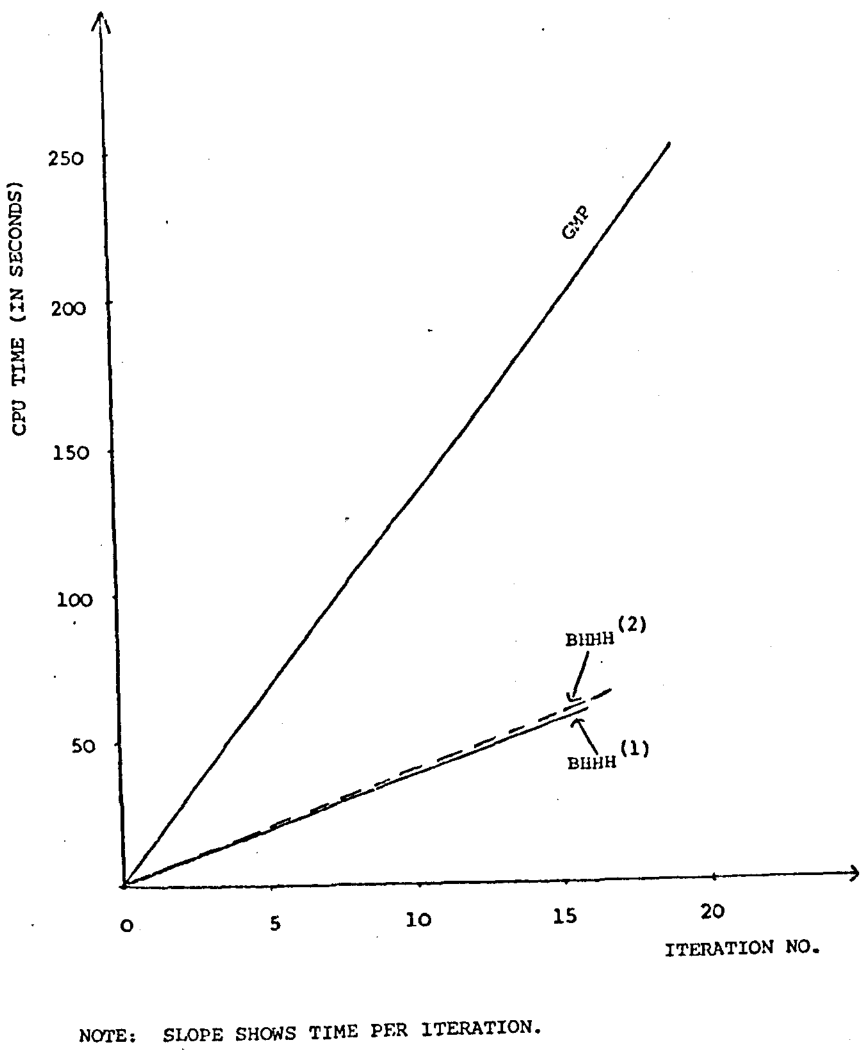


Figure 7.2

In Table 2b, BHHH$^{(1)}$ performs best, this is the only case where the old line search with step-size fixed to one works better than the modified line search. GMP seems to be slow for this model.

Tables 2c and 2d present very similar results except the CPU times for each method; notice that they have increased substantially.

Figure 7.2 shows the differences in terms of CPU times for the three methods with the true initial values.

(c) Model (iii), p = 6

Table 3a Final Estimates of Parameters

Parameters	Initial Values	BHHH(2) (Modified Line Search)	GMP(1) (Analytic Derivatives)	GMP(2) (Finite Differences)
γ	0.3	0.2973	0.2972	0.2972
α	1.0	0.9726	0.9728	0.9728
θ	1.0	1.0010	1.0010	1.0010
η	5.0	5.0012	5.0012	5.0012
η_{22}	5.0	4.9896	4.9896	4.9896
η_{44}	5.0	5.0000	4.9999	4.9999

Table 3b Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) seconds
BHHH(2)	10	12	-798.450121	-805.136759	16.8
GMP(1)	12	26	-798.450121	-805.136993	90.7
GMP(2)	18	229	-798.450121	-805.136993	227.0

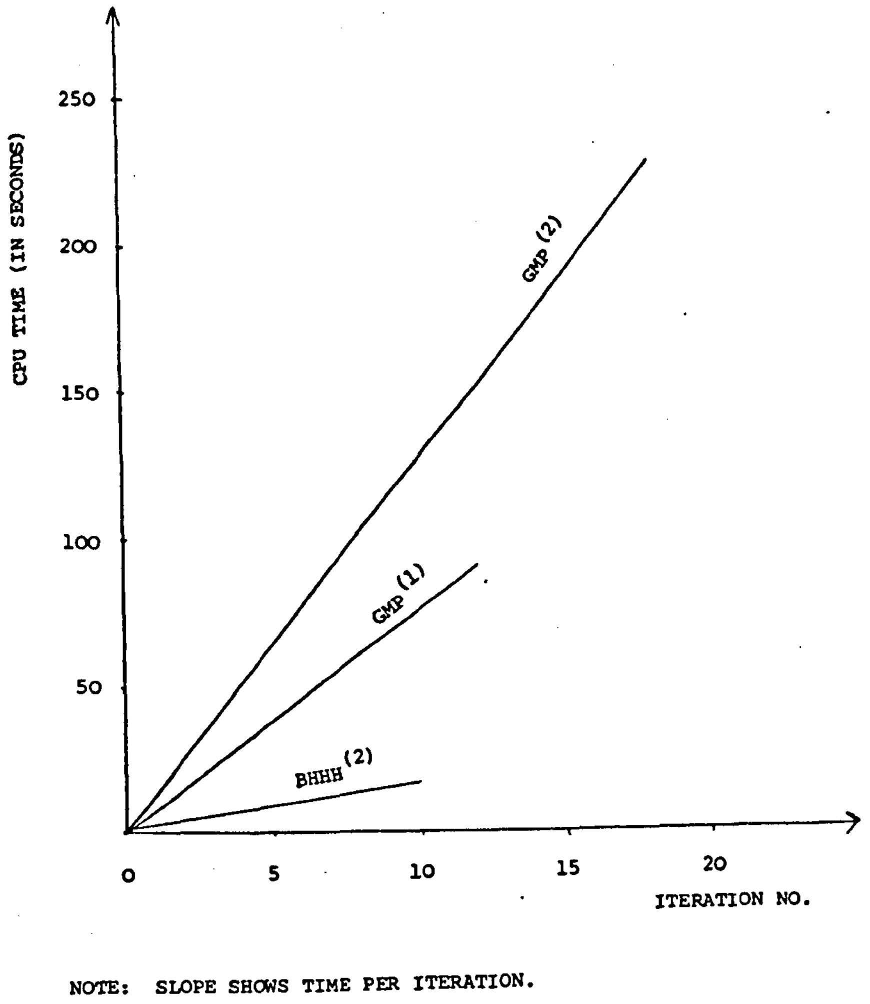


Figure 7.3

In Tables 3a and 3b, the estimated parameters and log L* seemed to agree with each other. But there are vast differences in CPU times. Again BHHH$^{(2)}$ is the best procedure and is faster than GMP$^{(1)}$ by a factor of 2½ to 3. Although GMP$^{(2)}$ converged to the same optimum, it is a highly inefficient method.

Figure 7.3 gives the CPU times against iteration numbers for the three estimation methods.

Note:

The above models were also tested with $\sigma^2 = 0.5$, the CPU time for each model was sufficiently large (> 600 seconds), yet the models did not seem to converge. Because of the huge CPU time further experimentation with large values of σ^2 for these three models is not feasible.

$n = 2$

For the $n = 2$ system, we present results for models (iv) to (vi) with $T = 50$, $\varepsilon = 1.0$, $\gamma_i = 0.5$, $\delta_i = 0.7$ and varying σ^2 from 0.1 to 0.5. Only BHHH with modified line search and GMP with analytical derivatives were considered for such experiments.

(d) Model (iv), $p = 9$

Table 4a Final Estimates of Parameters

Parameters	Initial Values	$\sigma^2 = 0.1$		$\sigma^2 = 0.2$		$\sigma^2 = 0.3$		$\sigma^2 = 0.5$	
		BHHH	GMP	BHHH	GMP	BHHH$^+$	GMP$^+$	BHHH^{++}	GMP
γ_1	0.5	0.9628	0.9628	1.2953	1.2952	1.5669	1.5661	2.0013	1.9866
γ_2	0.5	1.2352	1.2350	1.6225	1.6220	1.9466	1.9410	2.5182	2.4789
α_1	1.0	0.4627	0.4628	0.3919	0.3919	0.3627	0.3630	0.3367	0.3387
α_2	1.0	0.3794	0.3794	0.3298	0.3299	0.3053	0.3059	0.2775	0.2799
θ	1.0	0.9412	0.9412	0.9141	0.9140	0.8927	0.8920	0.8597	0.8563
δ_1	0.7	0.6737	0.6737	0.6665	0.6664	0.6621	0.6619	0.6572	0.6560
δ_2	0.7	0.6816	0.6816	0.6763	0.6763	0.6732	0.6729	0.6708	0.6689
η_{11}	5.0	4.6762	4.6760	4.5643	4.5639	4.4835	4.4788	4.3696	4.3450
η_{22}	5.0	5.0389	5.0387	5.0725	5.0721	5.1063	5.1008	5.1853	5.1538

Table 4b Details of Iterative Convergence

Method	σ^2	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH	0.1	51	112^{Δ}	-210.671923	-218.982182	76.8
GMP		55	81	-210.671923	-218.982182	112.0
BHHH	0.2	89	155^{Δ}	-176.010432	-184.440556	106.4
GMP		54	79	-176.010432	-184.440556	112.2
BHHH^{+}	0.3	87	166^{Δ}	-155.734175	-164.257193	120.0^{+}
GMP^{+}		52	75	-155.734175	-164.257211	120.0^{+}
BHHH^{++}	0.5	92	204^{Δ}	-130.188433	-138.861748	155.0^{++}
GMP		59	82	-130.188433	-138.862082	120.8

Notes: Notations used for models (iv) to (vi)

++ non-convergence after 100 iterations.

+ non-convergence after 120 seconds.

Δ number of function calls including the number of function evaluations in gradient check by numerical approximation.

(e) Model (v), p = 6

Table 5a Final Estimates of Parameters

Parameters	Initial Values	$\sigma^2 = 0.1$		$\sigma^2 = 0.2$		$\sigma^2 = 0.3$		$\sigma^2 = 0.5$	
		BHHH	GMP	BHHH	GMP	BHHH	GMP	BHHH	GMP
γ	0.5	1.0534	1.0534	1.3346	1.3346	1.5578	1.5569	1.9148	1.9134
α	1.0	0.4528	0.4528	0.3957	0.3958	0.3692	0.3693	0.3423	0.3424
θ	1.0	0.9361	0.9361	0.9101	0.9100	0.8896	0.8894	0.8565	0.8562
δ	0.7	0.6755	0.6755	0.6680	0.6680	0.6629	0.6629	0.6559	0.6558
η_{11}	5.0	4.6689	4.6689	4.5529	4.5530	4.4660	4.4646	4.3304	4.3284
η_{22}	5.0	4.9437	4.9437	4.9449	4.9449	4.9479	4.9466	4.9527	4.9508

Table 5b Details of Iterative Convergence

Method	σ^2	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH	0.1	45	70^{Δ}	-210.671923	-218.947553	34.0
GMP		26	38	-210.671923	-218.947553	44.0
BHHH	0.2	100	121^{Δ}	-176.010432	-184.409121	59.4
GMP		27	40	-176.010432	-184.409122	46.5
BHHH	0.3	52	77^{Δ}	-155.734175	-164.223673	37.9
GMP		26	39	-155.734175	-164.223674	47.5
BHHH	0.5	61	96^{Δ}	-130.188433	-138.820730	47.1
GMP		29	43	-130.188433	-138.820732	51.4

(f) Model (vi), $p = 4$

Table 6a Final Estimates of Parameters

Parameters	Initial Values	$\sigma^2 = 0.1$		$\sigma^2 = 0.2$		$\sigma^2 = 0.3$		$\sigma^2 = 0.5$	
		BHHH	GMP	BHHH	GMP	BHHH	GMP	BHHH	GMP
γ	0.5	0.9036	0.9036	1.0702	1.0702	1.1924	1.1923	1.3886	1.3887
α	1.0	0.3694	0.3694	0.3282	0.3282	0.3128	0.3128	0.2997	0.2996
θ	1.0	1.0471	1.0471	1.0651	1.0651	1.0784	1.0784	1.0996	1.0996
η	5.0	5.4046	5.4046	5.5691	5.5691	5.6950	5.6950	5.9013	5.9014

Table 6b Details of Iterative Convergence

Method	σ^2	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH	0.1	20	34^{Δ}	-210.671923	-217.132402	11.6
GMP		18	27	-210.671923	-217.132402	23.9
BHHH	0.2	25	76^{Δ}	-176.010432	-182.350609	25.6
GMP		19	34	-176.010432	-182.350609	30.0
BHHH	0.3	21	58^{Δ}	-155.734175	-161.997569	19.6
GMP		18	25	-155.734175	-161.997569	23.6
BHHH	0.5	23	69^{Δ}	-130.188433	-136.368487	23.3
GMP		20	39	-130.188433	-136.368487	30.6

Tables 4-6 show that the BHHH method is a more efficient procedure for the above models. When σ^2 is small (Tables 4a and 4b), the method works well but when σ^2 is increased to 0.5, then the GMP procedure performs better. In the case where $\sigma^2 = 0.3$, both methods fail to converge because the model is badly identified.

In Tables 5a and 5b, again BHHH is a better procedure for this set of models. Again in Tables 6a and 6b, BHHH performs best.

From the above experiments, the evidence is that BHHH is a better procedure for complicated models providing σ^2 is small. If we have a large σ^2, the procedure tends to be slow to locate the maximum of the likelihood function. For simple models (Tables 6a and 6b), both methods perform well but BHHH seems to be more efficient.

We now present some results of estimating models (iv) to (vi) by shifting the starting values of parameters and we take $\sigma^2 = 0.1$.

(g) $n = 2$, $p = 9$, $T = 50$, shifted initial values from true values.

Table 7a Final Estimates of Parameters

Parameters	Shifted Initial Values	BHHH$^+$ (Modified Line Search)	GMP (Analytical Derivatives)
γ_1	0.45	12.8520	0.9628
γ_2	0.45	57.5570	1.2350
α_1	0.95	0.0794	0.4628
α_2	0.95	0.0506	0.3794
θ	0.95	1.4448	0.9412
δ_1	0.65	0.8379	0.6737
δ_2	0.65	0.9728	0.6816
η_{11}	4.95	9.9421	4.6760
η_{22}	4.95	15.3090	5.0387

Table 7b Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH$^+$	81	163$^\Delta$	-133.414671	-197.331094	120.8$^+$
GMP	49	68	-133.414671	-218.982182	101.8

Note: Compare with Table 4a for $\sigma^2 = 0.1$, GMP tends to work well although the starting values are not close to the true values, in fact the run time is less than the case where we started the model with its true values. For BHHH it tends to locate a local maximum rather than the global maximum if the starting values are not close to the final estimate $\underline{\theta}^*$ for this particular model.

(h) $n = 2$, $p = 6$, $T = 50$, shifted initial values from true values.

Table 8a Final Estimates of Parameters

Parameters	Shifted Initial Values	BHHH (Modified Line Search)	GMP (Analytical Derivatives)
γ	0.45	1.0535	1.0534
α	0.95	0.4530	0.4528
θ	0.95	0.9361	0.9361
δ	0.65	0.6756	0.6755
η_{11}	4.95	4.6689	4.6689
η_{22}	4.95	4.9438	4.9437

Table 8b Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH	52	140^{Δ}	-133.414671	-218.947550	62.6
GMP	23	36	-133.414671	-218.947553	42.6

Note: Compare with Tables 5a and 5b for $\sigma^2 = 0.1$, GMP is more efficient in locating the maximum of the likelihood function although the starting values are shifted away from the true values. On the other hand, BHHH takes twice as long to converge compared with its previous CPU time.

(i) $n = 2$, $p = 4$, $T = 50$, shifted initial values from true values.

Table 9a Final Estimates of Parameters

Parameters	Shifted Initial Values	BHHH (Modified Line Search)	GMP (Analytical Derivatives)
γ	0.45	0.9036	0.9036
α	0.95	0.3694	0.3694
θ	0.95	1.0471	1.0471
η	4.95	5.4046	5.4046

Table 9b Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH	27	76^{Δ}	-135.783150	-217.132402	25.6
GMP	20	31	-135.783150	-217.132402	25.9

Note: Compare Table 9b with Table 6b for $\sigma^2 = 0.1$, the BHHH procedure takes twice as long to locate the same maximum when the starting values of the parameters are not close to the true values, but GMP works well althouth we have shifted the parameters.

The above experiments have provided us some evidence that the BHHH is sensitive over the starting values of the parameters. If the starting values of any models that are not close to the final estimates, it would be appropriate to use GMP and then go to BHHH.

To test the effect of sample size, we estimate model (ii) with T = 20. Tables 10a and 10b present the result from these runs.

Table 10a Final estimates of the Parameters

Parameters	Initial Values	BHHH (Modified line Search)	GMP (Analytical derivatives)
γ_1	0.3	0.3041	0.3042
γ_2	0.3	0.3516	0.3516
γ_3	0.3	0.3334	0.3334
γ_4	0.3	0.3153	0.3153
γ_5	0.3	0.3223	0.3223
α	1.0	0.9055	0.9054
θ	1.0	0.9942	0.9942
η_{11}	5.0	4.9816	4.9816
η_{22}	5.0	5.0018	5.0018
η_{33}	5.0	5.0053	5.0053
η_{44}	5.0	5.0028	5.0028
η_{55}	5.0	5.0015	5.0015

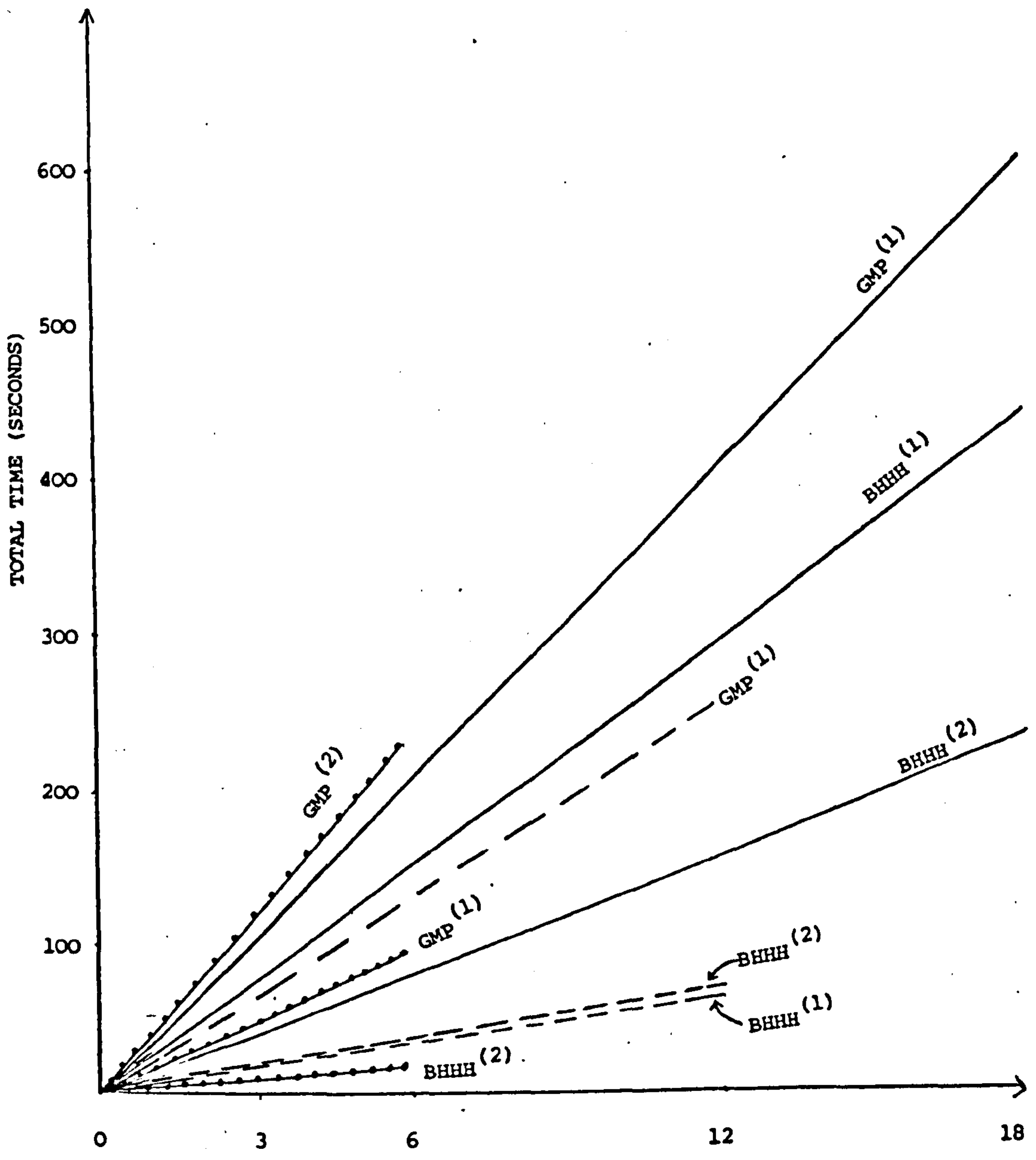
Table 10b Details of Iterative Convergence

Method	No. of Iterations	No. of Function Evaluations	Initial Value of Log L*	Final Value of Log L*	CPU Time (CDC 7600) Seconds
BHHH	44	69	-373.153883	-378.556694	66.5
GMP	25	53	-373.153883	-378.556694	112.1

If we compare Tables 10a and 10b with Tables 2a and 2b, the CPU time for BHHH method does not change much although we have reduced the sample size T from 50 to 20. But for GMP, the CPU time for $T = 20$ model has reduced substantially, this may indicate that the BHHH method will tend only to gain an advantage in time over the GMP when T is large.

Figures 7.4 and 7.5 show the time taken for each method against the number of parameters for models (i) to (iii) and (iv) to (vi) respectively. In all these cases (except model (ii)), BHHH with modified line search performs best, it is clearly more efficient when $p \geq 12$ (Figure 7.4). GMP (with numerical approximation to the derivatives) is not recommended when $p > 6$ (Figure 7.5).

Generally, BHHH seems to work well for this class of models, the drawback is that if u_t is not independently identically normally distributed, or if the form of the model is misspecified, which implies R (equation 3.16) is not a consistent positive definite estimator of the Hessian matrix H, then the method may not be efficient. But we need to stress that all methods are model dependent, and that it is difficult to predict their relative efficiencies. Both methods can be expected to obtain a relative maximum of the likelihood function if they converge. As a safeguard against lack of convergence it is suggested that the BHHH algorithm is tried with a limit on the number of iterations. If the method fails to converge, then the GMP algorithm is started from the final values achieved by the BHHH algorithm.



——— p = 18

------ p = 12

...... p = 6

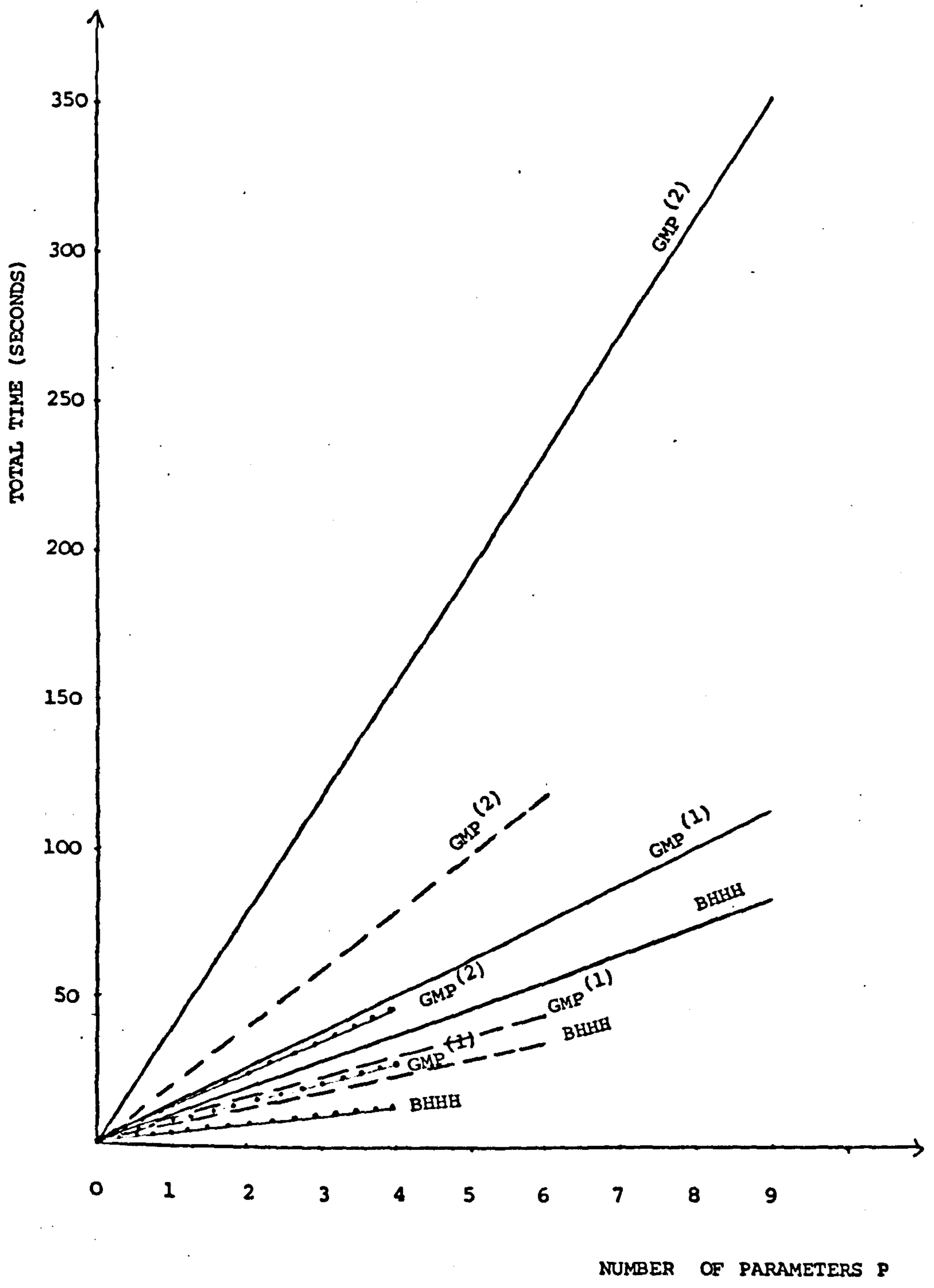
BHHH$^{(1)}$ ⟶ OLD LINE SEARCH

BHHH$^{(2)}$ ⟶ MODIFIED LINE SEARCH

GMP$^{(1)}$ ⟶ ANALYTICAL DERIVATIVES

GMP$^{(2)}$ ⟶ NUMERICAL APPROXIMATION

Figure 7.4



——— p = 9

------ p = 6

•••••• p = 4

BHHH ⟶ MODIFIED LINE SEARCH

GMP$^{(1)}$ ⟶ ANALYTICAL DERIVATIVES

GMP$^{(2)}$ ⟶ NUMERICAL APPROXIMATION

Figure 7.5

Non-Standard Models

The following table presents the results for model (v) by varying the parameter γ, $\sigma^2 = 0.005$.

We first choose $\gamma' = \gamma(1 + h)$ where $h = (-0.5, +0.5)$ and set $\gamma = 0.5$. We then generate the data series by using the true value of $\gamma = 0.5$ and set the initial values of γ' as defined above.

For 10 different starting points, we now have

$$\gamma' = \{.25, .30, .35, .40, .45, .55, .60, .65, .70, 75\}$$

and the parameter list beomces:

$$\underline{\theta}^{o} = \{\gamma, \alpha, \theta, \delta, \eta_{11}, \eta_{22}\}$$

Thus we have 10 models with $n = 2$, $p = 6$ and $T = 50$, each of these has a different starting value of γ'. The starting values of $\{\alpha, \theta, \delta, \eta_{11}, \eta_{22}\}$ are fixed at their true values, that is, $\{1.0, 1.0, 1.0, 5.0, 5.0\}$ respectively.

From Table 11, it can be seen that the CPU time for each run is large and hence we do not carry out the experiment further by varying the rest of the parameters.

Again we have found that BHHH works better except in the case $\gamma' = 0.45$.

Table 11

Final Estimates of Parameters and Details of Iterative Convergence

METHODS	γ^1	α	θ	δ	η_{11}	η_{22}	Log L^*	ITE No.	FUN EVALS.	CPU TIME
BHHH	0.4026	0.5663	0.9789	0.6909	4.8790	4.9666	-333.196186	21	52	26.4
GMP$^{(1)}$	0.4025	0.5660	0.9789	0.6909	4.8791	4.9665	-333.196220	19	30	39.2
GMP$^{(2)}$	0.4025	0.5660	0.9789	0.6909	4.8791	4.9665	-333.196220	22	216	95.3
BHHH	0.4501	0.6029	0.9786	0.6908	4.8772	4.9646	-333.326985	22	52	26.5
GMP$^{(1)}$	0.4501	0.6027	0.9786	0.6908	4.8771	4.9645	-333.326993	18	29	39.7
GMP$^{(2)}$	0.4501	0.6027	0.9786	0.6908	4.8771	4.9645	-333.326993	19	183	81.8
BHHH	0.4984	0.6333	0.9784	0.6908	4.8756	4.9630	-333.455264	18	45	22.9
GMP$^{(1)}$	0.4984	0.6334	0.9783	0.6907	4.8754	4.9629	-333.455282	19	30	42.2
GMP$^{(2)}$	0.4984	0.6334	0.9783	0.6907	4.8754	4.9629	-333.455282	23	225	97.5
BHHH	0.5470	0.6591	0.9781	0.6907	4.8742	4.9616	-333.581892	17	44	22.4
GMP$^{(1)}$	0.5471	0.6594	0.9781	0.6907	4.8740	4.9615	-333.581956	18	31	38.7
GMP$^{(2)}$	0.5471	0.6594	0.9781	0.6907	4.8740	4.9615	-333.581956	18	174	78.4
BHHH	0.5962	0.6818	0.9778	0.6906	4.8725	4.9601	-333.707470	17	40	41.7
GMP$^{(1)}$	0.5962	0.6817	0.9779	0.6906	4.8727	4.9603	-333.707476	18	30	20.4
GMP$^{(2)}$	0.5962	0.6817	0.9779	0.6906	4.8727	4.9603	-333.707476	20	195	87.0
BHHH	0.6949	0.7175	0.9775	0.6906	4.8708	4.9585	-333.955980	17	41	20.9
GMP$^{(1)}$	0.6948	0.7176	0.9775	0.6906	4.8708	4.9585	-333.955984	17	29	41.2
GMP$^{(2)}$	0.6948	0.7176	0.9775	0.6906	4.8708	4.9585	-333.955984	19	188	84.4
BHHH	0.7443	0.7325	0.9773	0.6905	4.8699	4.9576	-334.079198	13	34	17.4
GMP$^{(1)}$	0.7443	0.7324	0.9774	0.6905	4.8701	4.9578	-334.079223	17	29	36.7
GMP$^{(2)}$	0.7443	0.7324	0.9774	0.6905	4.8701	4.9578	-334.079223	21	211	92.6
BHHH	0.7940	0.7453	0.9773	0.6905	4.8698	4.9574	-334.201873	15	40	20.4
GMP$^{(1)}$	0.7940	0.7454	0.9772	0.6905	4.8695	4.9572	-334.201879	18	30	37.7
GMP$^{(2)}$	0.7940	0.7454	0.9772	0.6905	4.8695	4.9572	-334.201879	18	177	79.9
BHHH	0.8440	0.7571	0.9770	0.6905	4.8682	4.9563	-333.323967	14	35	17.8
GMP$^{(1)}$	0.8437	0.7570	0.9771	0.6905	4.8690	4.9567	-333.323996	17	30	37.6
GMP$^{(2)}$	0.8437	0.7570	0.9771	0.6905	4.8690	4.9567	-333.323996	20	200	89.6
BHHH	0.8937	0.7676	0.9770	0.6905	4.8686	4.9564	-334.445533	10	28	14.4
GMP$^{(1)}$	0.8934	0.7675	0.9770	0.6905	4.8686	4.9562	-334.445602	17	30	37.7
GMP$^{(2)}$	0.8934	0.7675	0.9770	0.6905	4.8686	4.9562	-334.445602	19	188	84.4

Note: BHHH with old line search
GMP$^{(1)}$ with analytical derivatives
GMP$^{(2)}$ with finite differences
CPU time is CDC 7600 time

7.7 Results and Timings for Model (iii) on the Distributed Array Processor

Five sets of model (iii) were tested. The model had 4096 observations. Due to its size it was not possible to run it on the CDC 7600 and ICL 2980 computers.

To provide a comparison with the DAP program, version (A), we ran the serial version (NLMLE) for 64, 128, 256, 512, 1024 and 2048 observations, respectively, and based on these timings we estimated the time for NLMLE on the 4096 observations.

Table 12 presents the timings of one function call for the above model with different sample sizes.

Table 12

T	ICL 2980 (Seconds)	CDC 7600 (Seconds)
64	5.444	1.196
128	11.248	2.370
256	19.737	4.698
512	38.384	9.311
1024	78.327	19.010
2048	174.691	42.401
4096	389.609*	93.691*

* Estimated Times

For each of version (B) and (C), we ran two models, the first having the starting values of the parameters as the true values, and the second having the starting values scaled by 2%. Table 13 presents the timings for all the models.

Table 13

Model	T	SYSTEM	NO. OF ITERATIONS	NO. OF FUNCTION CALLS	TIME PER ITERATION (SECONDS)	TOTAL CPU TIME (SECONDS)
1	4096	DAP	2	2	3.067	6.134
		ICL 2980	-	-	389.609*	-
		CDC 7600	-	-	93.691*	-
2	128	DAP	2	2	3.981	7.962
		ICL 2980	4	4	11.248	44.992
		CDC 7600	4	4	2.370	9.480
3	128^{+}	DAP	4	4	3.999	15.996
		ICL 2980	8	10	11.747	117.470
		CDC 7600	8	10	2.851	28.510
4	64	DAP	6	6	4.245	25.470
		ICL 2980	9	10	5.444	55.440
		CDC 7600	9	10	1.196	11.960
5	64^{+}	DAP	5	5	4.251	21.255
		ICL 2980	17	20^{Δ}	6.255	125.100^{Δ}
		CDC 7600	17	20^{Δ}	1.518	30.360^{Δ}

+ Scaled starting values of Parameters

* Estimates Times

Δ Non-convergence

If the timing is expressed graphically in Figure 7.6, we see that the DAP version (A) is faster than the serial version, on the CDC 7600, when $T \geq 179$, and, on the ICL 2980, when $T \geq 48$. Also in Figure 7.6, DAP versions (B) and (C) are slower than all the other versions for a single function call. However, during each function call in version (B) and (C), we are doing 64 and 32 simultaneous function evaluations respectively in the grid search procedure. In fact, from Table 13, the DAP versions (B) and (C) are more efficient at finding the optimum values of the parameters when the starting values are furthest from the true values.

Our conclusions based on the DAP programs are limited by the fact that the data for our comparisons was generated artificially. However, we would expect that the results for real data to be very similar. Figure 7.6 shows that DAP version (A) is very efficient for large sample models. Consequently, we would expect that the DAP would be appropriate for cross-section data models.

The application of a grid-search procedure in DAP versions (B) and (C) produced significant improvements for scaled starting values of the parameters. Thus we would expect similar improvements for real data sets.

Lastly, we would like to make some general remarks concerning the DAP. Clearly, the DAP should only be considered for a particular computation when the ability to do that computation on a serial computer is limited by the size of the data sets and the basic speed of the serial processor. For any particular computation there is no certainty that the DAP can provide a significant speed-up over a serial processor because the computation could be highly non-parallel.

In this section of the research, we have shown that non-linear optimisation does contain a signficant amount of parallel computation and hence the DAP should be seriously considered for this type of computation. To use the DAP rather than a serial computer requires the user to learn DAPFORTRAN. Since DAPFORTRAN is an extension of standard FORTRAN, this was a lot easier than learning a completely new language. Moreover, DAPFORTRAN was found to be more powerful and concise than standard FORTRAN. In fact, the conciseness of DAPFORTRAN enhanced the comprehension of the code and shortened the development time.

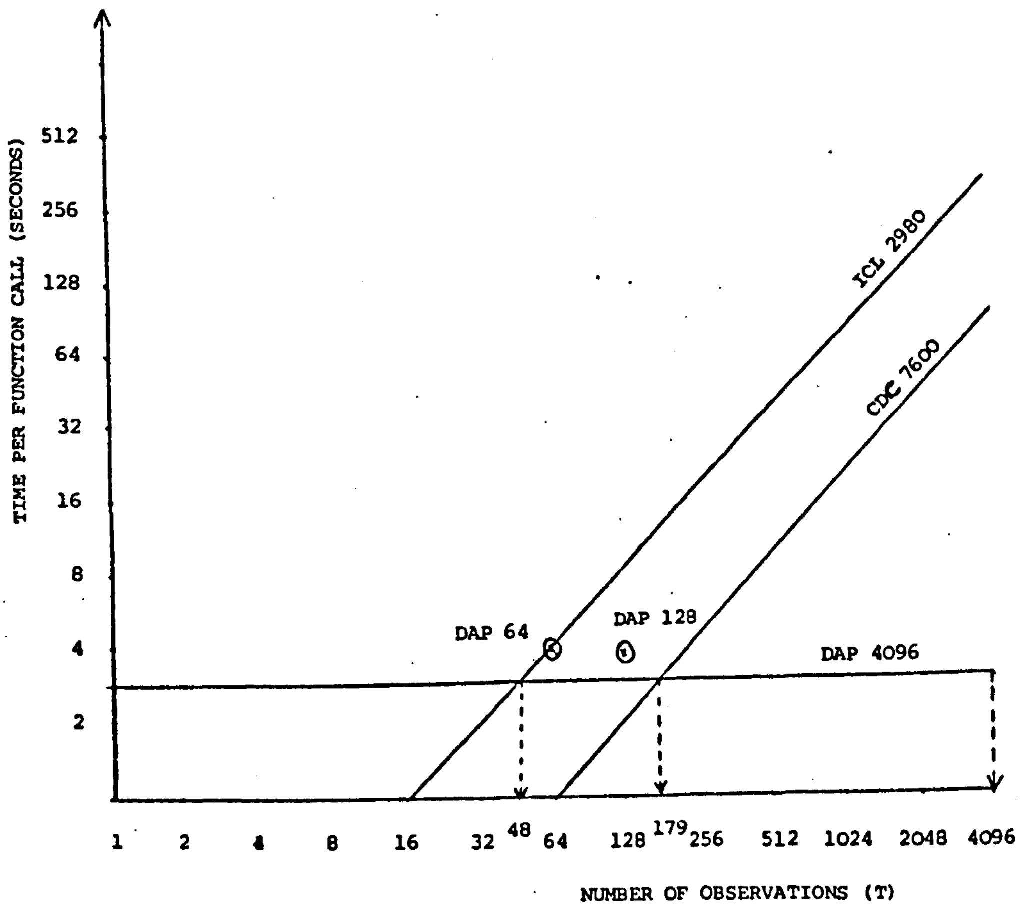


Figure 7.6

CHAPTER 8

AN AGGREGATE DEMAND MODEL FOR THE UNITED KINGDOM, 1957-1967

8. A Demand Model

A more realistic model used was a small macroeconomic model of the British Economy specified by David F. Hendry (1974). The model consists of eight equations, two of which are identities, and 18 unknown coefficients in its structural equations.

8.1 The Model (linear form)

In Hendry's specification, only equations linear in both variables and parameters are considred. The behavioural equations explain consumers' expenditure on durable goods (Cd) and all other goods and services (Cn), gross domestic fixed capital formation (I), inventory investment (Iv), and imports of goods and services (M). Gross domestic product (Y) is determined by the usual accounting identiy, and the model is closed by an empirical relation to determine disposable income (Yd). G is real current government expendtiure, X is real exports, T is real net indirect taxes, Pm is an index of relative import prices and N is a dummy variable related to the change in the timing of automobile licencing. Dummy variables for a constant term and three seasonal shift factors are included in every equation.

The FIML estimates are as follows:

(i) $Cd = 0.0816\ Yd + 57.0921\ N + 0.6530\ Cd_1 - 0.1898\ Cd_2 + u_1$

(ii) $Cn = 0.1458\ Yd + 0.7733\ Cn_1 + u_2$

(iii) $I = -\ 0.0690\ \Delta Y + 0.7439\ I_1 + 0.1042\ \Delta Y_1 + 0.2584\ I_2 + u_3$

(iv) $Iv = 0.1299\ \Delta Y + 0.4417\ Iv_1 + 0.2644\ Iv_2 + u_4$

(v) $M = 0.5004\ Iv - 4.8623\ Pm + 0.2338\ Y_1 + u_5$

(vi) $Yd = 0.2294\ Y + 0.7127\ Yd_1 + u_6$

$Y = Cd + Cn + I + Iv + G + X - T - M$

$\Delta Y = Y - Y_1$

The suffix is used to denote a corresponding lag, for example, $Cd_2 = Cd_{(t-2)}$.

Briefly, equation (i) is derived from a stock-adjustment, expected (or permanent) income model, and includes a dummy variable (N) for the annual vehicle registration letter. Equation (ii) is a transformed permanent income equation. Equations (iii) and (iv) are derived from flexible accelerator-capital stock adjustment models. Equation (v) assumes linear price, income, and stock building effects, and (vi) is a transformed distributed lag relationship.

It was decided as an exercise in estimating non-linear models to change only the first equation so that it is linear in the logarithms of the corresponding variables. In order to ensure that the model has, in fact, a predominantly non-linear form it was decided to use as its basic variables the logarithms of the economic variables.

8.2 Transformation of Model (non-linear form)

To transform the set of equations into non-linear form, we first transform the variable to logarithemic time series (except those variables with negative data) and then apply the exponential function to the transformed variables again. Hence we have a new set of equations that would correspond to equations (i) and (vi) but non-linear in both parameters and variables. To eliminate the two identities, we substitute both the variables Y and ΔY in the stochastic equations (i) to (vi).

Let the set of endogenous variables be:

$y_1 = \log Cd$

$y_2 = \log Yd$

$y_3 = \log Cn$

$y_4 = \log I$

$y_5 = Iv$

$y_6 = \log M$

and the set of exogenous variables be:

$z_1 = \log Cd_1$

$z_2 = \log Cd_2$

$z_3 = N$

$z_4 = \log Cn_1$

$z_5 = \log I_1$

$z_6 = \log I_2$

$z_7 = Iv_1$

$z_8 = \log Pm$

$z_9 = \log Yd_1$

$z_{10} = G + X - T$

$z_{11} = Y_1$

$z_{12} = Y_1 - Y_2$

$z_{13} = Iv_2$

Now the model becomes:

(i) $u_1 = y_1 - \beta_{12}y_2 - \gamma_{11}z_1 - \gamma_{12}z_2 - \gamma_{13}z_3 - \gamma_{10}$

(ii) $u_2 = \exp y_3 - \beta_{22} \exp y_2 - \gamma_{24} \exp z_4 - \gamma_{20}$

(iii) $u_3 = \exp y_4 - \beta_{38}\{\exp y_1 + \exp y_3 + \exp y_4 + y_5 - \exp y_6 + z_{10}$

$- z_{11}\} - \gamma_{35} \exp z_5 - \gamma_{36} \exp z_6 - \gamma_{3(12)}z_{12} - \gamma_{30}$

(iv) $$u_4 = y_5 - \beta_{48}\{\exp y_1 + \exp y_3 + \exp y_4 + y_5 - \exp y_6 + z_{10} - z_{11}\} - \gamma_{47}z_7 - \gamma_{4(13)}z_{13} - \gamma_{40}$$

(v) $$u_5 = \exp y_6 - \beta_{55}y_5 - \gamma_{58}\exp z_8 - \gamma_{5(11)}z_{11} - \gamma_{50}$$

(vi) $$u_6 = \exp y_2 - \beta_{67}\{\exp y_1 + \exp y_3 + \exp y_4 + y_5 - \exp y_6 + z_{10}\} - \gamma_{6(9)}z_9 - \gamma_{60}$$

We have a total of 24 unknown parameters (18 coefficients plus 6 constants) to be estimated in this transformed model.

8.3 Treatment of Coefficients for Equation u_1 and Constants for all Equations

Let $\bar{Y}_1 = \bar{C}d$

and $\bar{Y}_2 = \bar{Y}d$ where $\bar{C}d = \dfrac{\underset{t}{\Sigma} Cd}{T}$ and $\bar{Y}d = \dfrac{\underset{t}{\Sigma} Yd}{T}$.

Then to obtain starting values for the parameters we linearise the first equation in terms of the logarithmic variables by taking a first order Taylor series expansion of the FIML estimates equation in the form:

$$\exp y_1 = 0.0816 \exp y_2 + 52.091\, z_3 + 0.6530 \exp z_1 - 0.1898 \exp z_2 + u_1.$$

This gives $$\beta_{12} = \hat{\beta}_{12}\left(\frac{\bar{Y}_2}{\bar{Y}_1}\right),$$

where $\hat{\beta}_{12}$ is the FIML estimate of Yd in equation (i), that is, $\hat{\beta}_{12} = 0.0816$.

Let $\bar{z}_1 = \bar{C}d_1$, $\bar{z}_2 = \bar{C}d_2$, where $\bar{C}d_1 = \frac{\sum_t Cd_1}{T}$ and $\bar{C}d_2 = \frac{\sum_t Cd_2}{T}$

$$\text{then } \gamma_{11} = \hat{\gamma}_{11}\left(\frac{\bar{z}_1}{\bar{Y}_1}\right)$$

$$\gamma_{12} = \hat{\gamma}_{12}\left(\frac{\bar{z}_2}{\bar{Y}_1}\right)$$

$$\text{and } \gamma_{13} = \hat{\gamma}_{13}\left(\frac{1}{\bar{Y}_1}\right)$$

again $\hat{\gamma}_{11}$, $\hat{\gamma}_{12}$, $\hat{\gamma}_{13}$ are the FIML estimates of Cd_1, Cd_2 and N respectively.

The Hendry model includes seasonal dummies in each equation, which contributes 18 coefficients to the total of 36 parameters which he estimates. It was considered that 36 parameters were too many to estimate with the program in a full non-linear model, so that to reduce the number of parameters to 18 it would be better to deseasonalise the data, and omit the seasonal dummies from the equations. This required an adjustment to the starting values of the constant terms on the equations which were computed as follows:

$$\text{Let } W_1 = Y_1 - \beta_{12} Y_2 - \gamma_{11}z_1 - \gamma_{12}z_2 - \gamma_{13}z_3$$

and now calculate the quarterly means of

$\bar{W}_1(1)$ = first quarter mean of W_1

$\bar{W}_1(2)$ = second quarter mean of W_1

$\bar{W}_1(3)$ = third quarter mean of W_1

$\bar{W}_1(4)$ = forth quarter mean of W_1

and then take as initial values,

$$\gamma_{10} = \bar{W}_1(4)$$

$$\gamma_{1(14)} = \bar{W}_1(1) - \bar{W}_1(4)$$

$$\gamma_{1(15)} = \bar{W}_1(2) - \bar{W}_1(4)$$

$$\gamma_{1(16)} = \bar{W}_1(3) - \bar{W}_1(4).$$

Now we have the following starting values of all the constant coefficients:

For all the equations except equation (i), we have

$$\gamma^*_{i0} = \gamma_{i0} + \frac{1}{4}(\gamma_{i(14)} + \gamma_{i(15)} + \gamma_{i(16)}),$$

where γ_{i0}, $i = 1, \ldots, 6$ are the values of constants from the FIML estimates.

For equation (i), we calculate W_1 as before but now take γ^*_{i0} = Arithmetic mean of W_1 for the whole sample.

For the other unknown coefficients, the corresponding FIML estiamtes are taken as their starting values.

8.4 Deseasonised Data Series

Let $X_t = \log x_t = \alpha_o + \alpha_1 Q_{1t} + \alpha_2 Q_{2t} + \alpha_3 Q_{3t} + V_t$.

We choose the dummy variables to be Q_{1t}, Q_{2t} and Q_{3t} where:

Q_{1t}	Q_{2t}	Q_{3t}
3	-1	-1
-1	3	-1
-1	-1	3
-1	-1	-1
3	-1	-1
-1	3	-1
-1	-1	3
-1	-1	-1
⋮	⋮	⋮

and $t = 1, \ldots, T$.

Then the α_i are determined by multiple regression.

Now let

$$X_t^* = X_t - \alpha_1 Q_{1t} - \alpha_2 Q_{2t} - \alpha_3 Q_{3t}$$

and

$$Z^* = \begin{pmatrix} 1 & 3 & -1 & -1 \\ 1 & -1 & 3 & -1 \\ 1 & -1 & -1 & 3 \\ 1 & -1 & -1 & -1 \\ 1 & 3 & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

where the last three columns of Z^* are Q_{1t}, Q_{2t} and Q_{3t} respectively, then

$$\alpha = (Z^{*\prime}Z^*)^{-1}(Z^{*\prime}X),$$

where X is the data matrix.

Define

$$\alpha^+ = \begin{pmatrix} \alpha_1 & \cdots \\ \alpha_2 & \cdots \\ \alpha_3 & \cdots \end{pmatrix}$$

and $$Z^+ = \begin{pmatrix} Q_{1t} & Q_{2t} & Q_{3t} \\ \vdots & \vdots & \vdots \end{pmatrix}$$

then we have the adjusted data series of

$$X^* = X - Z^+\alpha^+ .$$

8.5 NLMLE Specifications of the Model

(i) parameter list

coefficients	β_{12}	β_{22}	β_{38}	β_{48}	β_{55}	β_{67}
NLMLE variables	v_1	v_2	v_3	v_4	v_5	v_6

coefficients	γ_{11}	γ_{12}	γ_{13}	γ_{24}	γ_{35}	γ_{36}
NLMLE variables	v_7	v_8	v_9	v_{10}	v_{11}	v_{12}

coefficients	$\gamma_{3(12)}$	γ_{47}	$\gamma_{4(13)}$	γ_{58}	$\gamma_{5(11)}$	γ_{69}
NLMLE variables	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}	v_{18}

coefficients	γ_{10}	γ_{20}	γ_{30}	γ_{40}	γ_{50}	γ_{60}
NLMLE variables	v_{19}	v_{20}	v_{21}	v_{22}	v_{23}	v_{24}

endogenous variables	y_1	y_2	y_3	y_4	y_5	y_6
NLMLE variables	v_{25}	v_{26}	v_{27}	v_{28}	v_{29}	v_{30}

exogenous variables	z_1	z_2	z_3	z_4	z_5	z_6	z_7
NLMLE variables	v_{31}	v_{32}	v_{33}	v_{34}	v_{35}	v_{36}	v_{37}

exogenous variables	z_8	z_9	z_{10}	z_{11}	z_{12}	z_{13}
NLMLE variables	v_{38}	v_{39}	v_{40}	v_{41}	v_{42}	v_{43}

Stochastic equations	u_1	u_2	u_3	u_4	u_5	u_6
NLMLE equations	F_1	F_2	F_3	F_4	F_5	F_6

(ii) Equations

The transformed stochastic equations become:

$$F_1 = v_{25} - v_1 * v_{26} - v_7 * v_{31} - v_8 * v_{32} - v_9 * v_{33} - v_{19}$$

$$F_2 = \text{EXP } v_{27} - v_2 * \text{EXP } v_{26} - v_{10} * \text{EXP } v_{34} - v_{20}$$

$$F_3 = \text{EXP } v_{28} - v_3 * (\text{EXP } v_{25} + \text{EXP } v_{27} + \text{EXP } v_{28} + v_{29} - \text{EXP } v_{30} + v_{40} - v_{41}) - v_{11} * \text{EXP } v_{35} - v_{12} * \text{EXP } v_{36} - v_{13} * v_{42} - v_{21}$$

$$F_4 = v_{29} - v_4 * (\text{EXP } v_{25} - \text{EXP } v_{27} + \text{EXP } v_{28} + v_{29} - \text{EXP } v_{30} + v_{40} - v_{41}) - v_{14} * v_{37} - v_{15} * v_{43} - v_{22}$$

$$F_5 = \text{EXP } v_{30} - v_5 * v_{29} - v_{16} * \text{EXP } v_{38} - v_{17} * v_{41} - v_{23}$$

$$F_6 = \text{EXP } v_{26} - v_6 * (\text{EXP } v_{25} + \text{EXP } v_{27} + \text{EXP } v_{28} + v_{29} - \text{EXP } v_{30} + v_{40}) - v_{18} * \text{EXP } v_{39} - v_{24}$$

8.6 Results

For the BHHH procedure, the model converged after 116 iterations with 222 function evaluations (Tables 1a and 1b).

log-likelihood function = - 639.6143

CPU time = 743 seconds (CDC 7600)

Table 1a

Coefficients	Starting Values	Parameter Estimates	Standard Errors	T-Ratios
β_{12}	0.9432	0.6417	0.6947	0.9237
β_{22}	0.1458	0.1276	0.0750	1.7016
β_{38}	-0.0690	-0.0796	0.1416	-0.5621
β_{48}	0.1299	0.0092	0.0292	0.3148
β_{55}	0.5004	0.4491	0.1629	2.7574
β_{67}	0.2294	0.3503	0.1467	2.3881
γ_{11}	0.6484	0.7271	0.2101	3.4609
γ_{12}	-0.1872	-0.1279	0.3822	-0.3345
γ_{13}	0.1374	0.1115	0.0566	1.9703
γ_{24}	0.7733	0.8061	0.1160	6.9483
γ_{35}	0.7439	0.7855	0.3609	2.1762
γ_{36}	0.2584	0.1974	0.3520	0.5607
$\gamma_{3(12)}$	0.1042	0.1104	0.1320	0.8361
γ_{47}	0.4417	0.3360	0.2349	1.4302
$\gamma_{4(13)}$	0.2644	0.3580	0.2592	1.3814
γ_{58}	-4.8623	-4.6153	5.0589	-0.9123
$\gamma_{5(11)}$	0.2338	0.2420	0.0442	5.4709
γ_{69}	0.7127	0.5673	0.1587	3.5742

Table 1b

Constants	Starting Values	Estimated Values
γ_{10}	2.2292	-3.0199
γ_{20}	235.5893	191.2679
γ_{30}	16.0904	36.7463
γ_{40}	13.5268	96.1541
γ_{50}	483.5083	417.2354
γ_{60}	58.2551	48.3693

NLMLE Estimates of the model are:

$$u_1 = \log Cd - 0.6417 \log Yd - 0.7271 \log Cd_1 + 0.1279 \log Cd_2 - 0.115\, N + 3.0199$$

$$u_2 = \exp(\log Cn) - 0.1276 \exp(\log Yd) - 0.8061 \exp(\log Cn_1) - 191.2679$$

$$u_3 = \exp(\log I) + 0.0796[\exp(\log Cd) + \exp(\log Cn) + \exp(\log I) + Iv - \exp(\log M) + (G + X - T) - Y_1] - 0.7855 \exp(\log I_1) - 0.1974 \exp(\log I_2) - 0.1104\,(Y_1 - Y_2) - 36.7463$$

$$u_4 = Iv - 0.0092[\exp(\log Cd) + \exp(\log Cn) + \exp(\log I) + Iv - \exp(\log (M) + (G + X - T) - Y_1] - 0.3360\, Iv_1 - 0.3580\, Iv_2 - 96.1541$$

$$u_5 = \exp(\log M) - 0.4491\, Iv + 4.6153 \exp(\log Pm) - 0.2420\, Y_1 - 417.2354$$

$$u_6 = \exp(\log Yd) - 0.3503[\exp(\log Cd) + \exp(\log Cn) + \exp(\log I) + Iv - \exp(\log M) + (G + X - T)] - 0.5673 \exp(\log Yd_1) - 48.3693$$

For the method of GMP with analytical derivatives (NAG), the model converged after 242 iterations with 284 function evaluations.

log-likelihood function = - 639.6141

CPU time = 2068 seconds (CDC 7600)

The estimated parameters (with the same starting values as BHHH) are shown in Table 2a and the estimated constants in Table 2b.

Table 2a

Coefficients	Parameter Estimates
β_{12}	0.6401
β_{22}	0.1268
β_{38}	-0.0803
β_{48}	0.0092
β_{55}	0.4468
β_{67}	0.3523
γ_{11}	0.7275
γ_{12}	-0.1272
γ_{13}	0.1114
γ_{24}	0.8074
γ_{35}	0.7864
γ_{36}	0.1966
$\gamma_{3(12)}$	0.1105
γ_{47}	0.3365
$\gamma_{4(13)}$	0.3568
γ_{58}	-4.6243
$\gamma_{5(11)}$	0.2420
γ_{69}	0.5659

Table 2b

Constants	Estimated Values
γ_{10}	-3.0168
γ_{20}	190.2829
γ_{30}	36.5368
γ_{40}	96.2071
γ_{50}	418.3268
γ_{60}	43.3531

From the results, if we compare the CPU times, the BHHH procedure seems to be a more efficient method than GMP. For this particular model, it is faster than GMP by a factor of 2½ in terms of computational time.

The log-likelihood function values and the parameter estimates of the two methods are reasonably close and give evidence that the model does converge to a strong local optimum. The time taken to converge for this model is sufficiently large as to discourage much experimentation with models of this size.

CHAPTER 9

GENERAL CONCLUSION

In this research, we have successfully developed a general differentiation program and applied it to non-linear econometric models. In particular, an estimation program (NLMLE) was written to estimate non-linear simultaneous equation systems. A serial version of this program was implemented on the CDC 7600 and ICL 2980 computers.

In order to improve the efficiency and decrease the computational time, a parallel version of the BHHH method was developed on the ICL DAP. In the course of this, three versions of the estimation program were designed which exploited the DAP architecture and at the same time improved the efficiency compared with the serial version. The three parallel versions were:

(i) A matrix mode implementation for models with up to 4096 observations.

(ii) A vector mode implementation for models up to 64 observations.

(iii) A matrix and vector modes implementation for models with between 65 and 128 observations.

For versions (ii) and (iii), the DAP was 'partitioned' into 64 and 32 'parallel processors', respectively, according to the number of observations. The advantage of doing this was to allow us to evaluate multiple step-sizes simultaneously in the line search during the optimisation porcedure. Hence the number of function calls was only one per interation; the algorithm also determines the best likelihood function value with the optimum step-size in one function call.

We have demonstrated that the DAP is relatively more efficient when the sample size of the model increases. The optimum performance was for models having close to 4096 observations. For this the DAP was approximately 30 times faster than the CDC 7600 and 127 times faster than the ICL 2980 computers. The most suitable application for such classes of models are panel data with large numbers of members of the sample in each cross-section.

Although in versions (ii) and (iii), the DAP time per function call was longer than the serial version, we were able to evaluate multiple step-sizes in the line search simultaneously. This meant we were able to reduce the number of iterations required for the model to converge since we could always locate the optimum step-size with the least function value (minimisation). If a model is not well behaved or the starting values of the parameter estimates are too far from the optimum, then it may take many iterations and function evaluations to converge, but on the DAP we showed that the time on each iteration could be much reduced by using multiple steps.

The serial version of the program worked well on the class of non-linear econometric models used to test the method. The function specification of the differentiation program enabled us to define any econometric functions whether they were non-linear in parameters, variables, or both. Arithmetic functions such as LOG, EXP, SINE, COSINE and ARC-TANGENT were provided. Thus it avoided the task of data transformation or parameter mapping.

The differentiation program provided analytic derivatives of the log-likelihood function which could be applied in a gradient-type or quasi-Newton type optimisation procedure. Also the modified one-dimensional line search procedure was very efficient compared with other methods (see Chapter 2) and the various gradient stopping criteria helped to improve the efficiency of the estimation program.

We have also demonstrated that the BHHH method was relatively more efficient for the class of models we have tested. When the size of the model increased and the model became more complex, the BHHH method performed better than the GMP (analytical derivatives). So the BHHH method generally worked well when:

(i) the sample size was large;

(ii) the error variance σ^2 was relatively small;

(iii) the model was complex and the parameter set was reasonably large;

(iv) the model was correctly specified;

(v) the starting values $\underline{\theta}^{(o)}$ must be close to $\underline{\theta}^*$.

Generally, for this class of models, the BHHH performed best, the GMP (with analytic derivatives) came second and GMP with numerical approximation to the derivatives performed worst. We recommend using BHHH or GMP if the analytic gradient of the log-likelihood function can be obtained easily. When the model is complex, BHHH would be a better choice.

Lastly, as we expected the BHHH method worked equally as well for other classes of model (see Chapter 8).

Thus we have written an efficient estimation program for general non-linear econometric models.

To improve the performance and efficiency of this program (perhaps for future research), we would suggest simplifying some derivative functions generated from the differentation program. This will avoid unnecessary repetitive calculations. Although we have done some simplification, these were relatively simple and trivial cases. A good, general and effective simplification routine would help to reduce the computational time substantially.

Another suggestion for the improvement is by using random directions in the DAP program. DAP is efficient at locating the optimum direction with the optimum step to give the optimum function value. All these could be done in parallel.

One final suggestion is to derive a completely new estimation procedure that would increase the degree of parallelism on the DAP. Research of this kind has been going on, especially on a variable-metric method.

It is our hope that ICL will build a 8 Mbyte DAP in the future. If this were done we could estimate a wider range of non-linear models, and perhaps by then, we could do more parallel computations on this kind of application.

It is also hoped that we can extend the present serial version of the estimation program, for example, by inserting some statistical tests. It might be worthwhile to program other parametric estimators such as non-linear three stage least squares.

APPENDIX A

Cholesky Factorisation

Consider the Cholesky factors of a modified matrix $H^{(k+1)}$ given by

$$H^{(k+1)} = H^{(k)} + \Pi_1 z^{(k)} z^{(k)'} + \Pi_2 \omega^{(k)} \omega^{(k)'} \tag{A1}$$

We consider the case using the modification

$$\begin{aligned} H^{(k+1)} &= H^{(k)} + \sigma z^{(k)} z^{(k)'} \\ &= L^{(k)} D^{(k)} L^{(k)'} + \sigma z^{(k)} z^{(k)'} \end{aligned} \tag{A2}$$

The diagonal elements of D will be denoted by $d_1, d_2, \ldots, d_n$.

Given that the initial estimate of H is positive definite, then the succeeding estimates are also positive definite regardless of the rounding error incurred. Two points must be emphasised:

(a) Unless $H^{(k+1)}$ is positive definite the Cholesky factorisation need not exist.

(b) Even if the Cholesky factorisation does not exist the numerical stability of any algorithm for modifying the triangular factors cannot be guaranteed when $H^{(k+1)}$ is indefinite. Thus it is generally unsatisfactory to modify the Cholesky factors and then alter any negative elements a-posteriori since the accuracy of the factorisation could be in doubt.

Equation (A2) could be written as:

$$H^{(k+1)} = L^{(k)}D^{(k)\frac{1}{2}}(I + \sigma VV')D^{(k)\frac{1}{2}}L^{(k)'} \qquad \text{(A3)}$$

where

$$L^{(k)}D^{(k)\frac{1}{2}}V = z^{(k)}$$

To avoid the calculation of square roots, a new $\tilde{V}$ is defined by the solution of the system of equations

$$L^{(k)}\tilde{V} = z^{(k)}$$

so that

$$\tilde{V} = D^{(k)\frac{1}{2}}V$$

Equation (A3) can further be written in the form

$$H^{(k+1)} = L^{(k)}D^{(k)\frac{1}{2}}A^{(1)}A^{(1)}D^{(k)\frac{1}{2}}L^{(k)'} \qquad \text{(A4)}$$

where

$$A^{(1)} = I - \sigma^{(1)}V^{(1)}V^{(1)'}$$

Define $V^{(j)}$ as the $(n-j+1) \times 1$ vector of the last $n-j+1$ elements of V $(V^{(1)} = V)$. This implies that

$$\sigma^{(1)} = \frac{1 \pm (1 + \sigma V'V)^{\frac{1}{2}}}{V'V}$$

provided the square root is real. The negative sign is always chosen since $A^{(1)}$ is then positive definite. The equation $\sigma^{(1)}$ can be equivalently written as

$$\sigma^{(1)} = -\frac{\sigma}{1 + (1 + \sigma\tilde{V}'[D^{(k)}]^{-1}\tilde{V})^{\frac{1}{2}}} \qquad (A5)$$

In the next $n-1$ steps $A^{(1)}$ is reduced to lower-triangular form by a sequence of orthogonal matrices $w^{(j)}$, $J = 1, 2, \ldots, n-1$, such that

$$\hat{L}^{(k)} = A^{(1)}W^{(1)}W^{(2)}, \ldots, W^{(n-1)}$$

where $\hat{L}^{(k)}$ is a lower-triangular matrix. Such a reduction can be achieved by the use of elementary Hermitian matrices of the form

$$W^{(j)} = I - \tau^{(j)} \left[\begin{array}{c} 0 \\ \hline u^{(j)} \end{array}\right] \left[\begin{array}{c|c} 0 & u^{(j)'} \end{array}\right]$$

with $u^{(j)}$ an $(n-j+1) \times 1$ vector and

$$\tau^{(j)} = {}^{2}/_{u^{(j)'}u^{(j)}}$$

For a general matrix A, with elements a_{ij}, the first stage of the reduction process is defined by the equations

$$u^{(1)'} = (a_{11} \pm \gamma^{(1)}, a_{12}, a_{13}, \ldots, a_{1n})$$

where

$$\gamma^{(1)^2} = \sum_{j=1}^{n} a_{ij}^2$$

and hence

$$\tau^{(1)} = (\gamma^{(1)^2} \pm \gamma^{(1)} a_{11})^{-1}$$

The first row of $AW^{(1)}$ is then of the form $(\pm \gamma^{(1)}, 0, \ldots, 0)$. If these results are applied to the special case of the matrix $A^{(1)}$ under consideration, the first stage of the desired reduction process is

$$\tau^{(1)} = \{\gamma^{(1)^2} \pm \gamma^{(1)} \theta^{(1)}\}^{-1}$$

where

$$\theta^{(1)} = 1 - \sigma^{(1)} v_1^2$$

$$= 1 - \sigma^{(1)} d_1^{-1} \tilde{v}_1^2$$

and

$$\gamma^{(1)^2} = \sigma^{(1)^2} v_1^2 \sum_{j=2}^{n} v_j^2 + \theta_1^{(1)^2}$$

$$= \sigma^{(1)} \tilde{v}_1^2 d_1^{-1} \sum_{j=2}^{n} d_j^{-1} \tilde{v}_j + \theta^{(1)^2}$$

The elements of $u^{(1)}$ are by definition

$$u_1^{(1)} = \theta^{(1)} \pm \gamma^{(1)}$$

$$u_j^{(1)} = - \sigma^{(1)} v_1 v_j \qquad j = 2, 3, \ldots, n$$

The sign before $\gamma^{(1)}$ is always chosen to be the same as that of $\theta^{(1)}$ so as to minimise rounding error.

$A^{(1)}W^{(1)}$ is of the form:

$$A^{(1)}W^{(1)} = \left[\begin{array}{c|c} \pm\gamma^{(1)} & 0 \\ \hline \beta^{(1)}v^{(2)} & A^{(2)} \end{array}\right]$$

where

$$A^{(2)} = I_{n-1} - \sigma^{(2)}v^{(2)}v^{(2)'}$$

with

$$\sigma^{(2)} = \sigma^{(1)}\{1 + v_1\tau^{(1)}\sigma^{(1)}(v_1 + v^{(1)'}u^{(1)})\}$$

$$= \tau^{(1)}\sigma^{(1)}(1 \pm \gamma^{(1)})$$

Similarly $\beta^{(1)}$ can be shown to be

$$\beta^{(1)} = -\sigma^{(1)}v_1 + \tau^{(1)}\sigma^{(1)}v_1\mu_1^{(1)} + \mu_1^{(1)}\tau^{(1)}\sigma^{(1)}v^{(1)'}u^{(1)} \qquad \text{(A6)}$$

$$= v^{(1)'}u^{(1)}\sigma^{(2)}$$

$$= \frac{d_1^{-\frac{1}{2}}}{\pm\gamma_1\tilde{v}_1}(1-\gamma^2)$$

which can be written as

$$\beta^{(1)} = d_1^{-\frac{1}{2}}\tilde{\beta}^{(1)}$$

Note that if $\tilde{v}_1 = 0$ then equation (A6) implies that $\tilde{\beta}^{(1)} = 0$.
Also note that μ_j is an element of u.

During the algorithm only $\tilde{\beta}^{(1)}$ need be calculated. Post-multiplication by $W^{(j)}$, $j = 2, \ldots, n$, leaves the first row and column of $A^{(1)}W^{(1)}$ unaltered. Extending the definitions of $\tilde{\beta}^{(1)}$ and $\gamma^{(1)}$ to $\tilde{\beta}^{(j)}$ and $\gamma^{(j)}$ respectively, $H^{(k+1)}$ can be written as

$$H^{(k+1)} = L^{(k)}D^{(k)^{\frac{1}{2}}}\hat{L}^{(k)}\hat{L}^{(k)'}D^{(k)^{\frac{1}{2}}}L^{(k)'}$$

where

$$\hat{L}^{(k)} = \left[\begin{array}{c|c|c|c} \pm\gamma^{(1)} & 0 & \cdots & 0 \\ \hline & \pm\gamma^{(2)} & & \vdots \\ \cline{2-2} d_1^{-\frac{1}{2}}\tilde{\beta}^{(1)}v^{(2)} & d_2^{-\frac{1}{2}}\tilde{\beta}^{(2)}v^{(3)} & & 0 \\ \cline{4-4} & & \cdots & \pm\gamma^{(n)} \end{array}\right]$$

which leads to

$$D^{(k)^{\frac{1}{2}}}\hat{L}^{(k)} = \left[\begin{array}{c|c|c|c} 1 & 0 & \cdots & 0 \\ \hline & 1 & & \vdots \\ \cline{2-2} \dfrac{\tilde{\beta}^{(1)}\tilde{v}^{(2)}}{\gamma^{(1)}d_1} & \dfrac{\tilde{\beta}^{(2)}\tilde{v}^{(3)}}{\gamma^{(2)}d_2} & & 0 \\ \cline{4-4} & & \cdots & 1 \end{array}\right] \left[\begin{array}{cccc} \pm\gamma^{(1)}d_1^{\frac{1}{2}} & 0 & \cdots & 0 \\ 0 & \pm\gamma^{(2)}d_2^{\frac{1}{2}} & & \vdots \\ \vdots & \cdots & \cdots & 0 \\ 0 & \cdots & 0 & \pm\gamma^{(n)}d_n^{\frac{1}{2}} \end{array}\right]$$

This will be written as

$$D^{(k)^{\frac{1}{2}}} \hat{L}^{(k)} = \tilde{L}^{(k)} D^{(k+1)^{\frac{1}{2}}}$$

Then

$$H^{(k+1)} = L^{(k)} \tilde{L}^{(k)} D^{(k+1)} \tilde{L}^{(k)'} L^{(k)'}$$

so that the required $L^{(k+1)}$ is given by

$$L^{(k+1)} = L^{(k)} \tilde{L}^{(k)}$$

The general $L^{(k)}$ and $\tilde{L}^{(k)}$ are dense lower-triangular matrices and straightforward multiplication would require $n^3/6 + O(n^2)$ multiplications. The method described above requires $3n^2/2 + O(n)$ multiplications to obtain the modified factors.

It is clear that the matrix $H^{(k+1)}$ will be positive definite unless $\sigma^{(1)}$ given by equation (A5) is imaginary. In this case two possible strategies can be followed to give a positive definite of $H^{(k+1)}$:

(i) The parameter σ can be made less negative.

(ii) The size of the diagonal elements of D can be increased.

A convenient modification of the formula for σ_1 amount to alter $H^{(k+1)}$ using (i) and (ii) can be determined from the expression

$$\sigma^{(1)} = - \frac{\sigma}{1 + (1 + \sigma \tilde{V}' [D^{(k)}]^{-1} \tilde{V})^{\frac{1}{2}}}$$

APPENDIX B

NLMLE Listing

```
      PROGRAM FIMLX
      LOGICAL IEND
      LOGICAL IREC,LTHETA,JACOB
      LOGICAL DERIV,DERCUV,SUCCESS
      INTEGER*8 ITIME
      INTEGER IIFLAG,IRESULT
      COMMON X(100,50)
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      COMMON /A8/ RES(20,20)
      COMMON /NAMES/ NAME(20)
      REAL NDERS,NDERJS
      DIMENSION V(24),VMUS(24)
      DIMENSION DELTA(50),HESL(276),HESD(50),W(145),GR(50)
      DIMENSION ITEXT(80)
      DIMENSION ISYM(200)
      EXTERNAL BHHH,EO4EAZ
      EXTERNAL FUNML,FUNSET,MONIT
      LOGICAL LOADLD
      IIFLAG=0
C
C             IMETH = 0     BHHH
C             IMETH = 1     GMP   ANALYTICAL DERIVATES
C             IMETH = 2     GMP   NUMERICAL APPROXIMATION
C
C             ISTEP = 0     GSTEP
C             ISTEP = 1     BARD
C
      CALL QMCMILLTIME(IIFLAG,ITIME,IRESULT)
      READ(5,10) IMETH,ISTEP
   10 FORMAT(20I4)
      MAXF=0
      NFUNC=0
      KC=0
      IADC=1
      IRAN=0
      MAXCON=0
      LTHETA=.FALSE.
      JACOB=.FALSE.
      READ(5,11) NB,NI,NINTF,NY,NZ,NPARAM,NT,NL,NR,NTRAN
   11 FORMAT(20I4)
      READ(5,151) (NAME(J),J=1,NPARAM)
  151 FORMAT(20A4)
      NQ=NB+NI
      NA=NT-NL
      NOAP1=NL+1
      CALL INPUT(NA,NOAP1,NVAR,NR,NTRAN)
      WRITE(6,100) NQ,NA,NL,NPARAM
  100 FORMAT(1HO,I4,' EQUATIONS',I8,' OBSERVATIONS',I8,' LAGS',I8,' PARA
     IMETERS')
     IMETERS')
C
C          READ IN INITIAL VALUES OF PARAMETERS
C          PUT PARAMETERS,ENDOGENOUS VARIABLES IN VECTOR
C
      READ(5,12) (V(I),I=1,NPARAM)
   12 FORMAT(8F10.4)
      IPARAM=NPARAM+NY
      DO 105 I=1,IPARAM
  105 IVECT(I)=I
      WRITE(6,107) (V(I),I=1,NPARAM)
  107 FORMAT(1HO,'  COEFFICIENTS   '/1HO,(8F16.5))
      IF(NQ .LE. 20) NFUNC=20
      NADMAX=1
      NS=NQ
      IF(NINTF .NE. 0) NS=NQ+NINTF
      DO 106 N=1,NS
      CALL RDCARD(ITEXT)
      CALL FRML(ITEXT,NFUNC,N,IADC,IEND,MAXCON,MAXF,KC,ISYM)
      IK=IADC-1
      LISTEN(N)=IK
      WRITE(6,200) (NLIST(J),J=NADMAX,IK)
  200 FORMAT(1H ,30I4)
      NADMAX=IADC
      IF(KC .EQ. 0) GO TO 104
      JC(N)=KC
      KC=0
      GO TO 106
  104 JC(N)=0
      KC=0
  106 CONTINUE
      ICON(1)=MAXCON
      NS=NQ
      IF(NINTF .NE. 0) NS=NQ+NINTF
      MAXAD=LISTEN(NS)
      IF(IMETH .GT. 0) GO TO 405
      CALL QMCMILLTIME(IIFLAG,ITIME,IRESULT)
      WRITE(6,99) ITIME
      CALL BHHH(NPARAM,V,VMUS)
      CALL QMCMILLTIME(IIFLAG,ITIME,IRESULT)
      WRITE(6,99) ITIME
      STOP
  405 N=NPARAM
      SMALL=SQRT(X02AAF(XTOL))
      DO 410 I=1,NPARAM
  410 DELTA(I)=SMALL
      ICOUNT=1
      IFAIL=0
      LOADLD=.TRUE.
      XTOL=0.001
      ETA=0.9
      STPMAX=1.0
      IL=N*(N-1)/2
      IW=7*N+1
      IWW=6*N+1
      MAXCAL=500
      IPRINT=1
      CALL QMCMILLTIME(IIFLAG,ITIME,IRESULT)
      WRITE(6,99) ITIME
99    FORMAT(1HO,'TIME = ',I20)
      CALL FUNML(NPARAM,V,FUN)
      ICOUNT=ICOUNT+1
      FUN=FUN-0.8*(ABS(FUN))
      IF(IMETH .GT. 1) CALL EO4CDF(NPARAM,V,FUN,GR,HESL,IL,HESD,LOADLD,
     IXTOL,DELTA,ETA,STPMAX,W,IW,FUNML,FUNSET,MONIT,IPRINT,MAXCAL,
     IIFAIL)
      IF(IMETH .EQ. 1) CALL EO4DDF(NPARAM,V,FUN,VMUS,HESL,IL,HESD,
     LLOADLD,XTOL,EO4EAZ,ETA,STPMAX,W,IWW,FUNML,BHHH,MONIT,IPRINT,
     LMAXCAL,IFAIL)
      CALL QMCMILLTIME(IIFLAG,ITIME,IRESULT)
      WRITE(6,99) ITIME
      IF(IMETH .GT. 1) WRITE(6,430) (GR(I),I=1,NPARAM)
  430 FORMAT(1HO,'DERIVATIVE FROM G-M'/1X,12F10.6)
      IF(IFAIL .EQ. 0) GO TO 436
      WRITE(6,431)
  431 FORMAT(//,1X,'ERROR EXITS FROM NAG ROUTINE BECAUSE')
      GO TO(415,416,417,418),IFAIL
  415 WRITE(6,432)
  432 FORMAT(1HO,'A PARAMETER IS OUTSIDE IST EXPECTED RANGE')
      GO TO 436
  416 WRITE(6,433)
  433 FORMAT(1HO,'MAXIMUM NUMBER OF ITERATIONS EXCEEDED')
      GO TO 436
  417 WRITE(6,434)
  434 FORMAT(1HO,'THE ALGORITHM DOES NOT SEEM TO BE CONVERGING')
      GO TO 436
  418 WRITE(6,435)
  435 FORMAT(1HO,'INITIAL SETTING OF FUNCTION SEEMS UNRELIABLE')
  436 WRITE(6,437) (V(I),I=1,NPARAM)
  437 FORMAT(' PARAMETER ESTIMATES'/(8X,10F12.6))
      WRITE(6,438) FUN
  438 FORMAT(1HO,'LOG LIKELIHOOD FUNCTION = ',F12.6)
      STOP
      END




      SUBROUTINE FUNSET(NPARAM,V,STEPC,FVEC)
      DIMENSION V(NPARAM),FVEC(NPARAM),STEPC(NPARAM)
      DO 20 I=1,NPARAM
      STORE=V(I)
      V(I)=V(I)+STEPC(I)
      CALL FUNML(NPARAM,V,FUN)
      FVEC(I)=FUN
      V(I)=STORE
   20 CONTINUE
      RETURN
      END
      SUBROUTINE MONIT(NPARAM,V,FUN,GR,HES,IL,HED,NCALL)
      DIMENSION V(NPARAM),GR(NPARAM),HED(NPARAM),HES(IL)
      IF(NCALL .EQ. 0) GO TO 10
      WRITE(6,2) NCALL
    2 FORMAT(1H0,' AFTER ',I5,' FUNCTION CALLS')
      GO TO 20
   10 WRITE(6,1)
    1 FORMAT(1H0,' FINAL SOLUTION IS ')
   20 WRITE(6,3) (V(I),I=1,NPARAM)
    3 FORMAT(1H0,' PARAMETER ESTIMATES'/(8X,10F10.6))
      GNORM=0.0
      BIG=HED(1)
      SMALL=BIG
      DO 30 I=1,NPARAM
      D1=HED(I)
      GNORM=GNORM+GR(I)*GR(I)
      IF(D1 .GT. BIG) BIG=D1
      IF(D1 .LT. SMALL) SMALL=D1
   30 CONTINUE
      GNORM=SQRT(GNORM)
      WRITE(6,35) GNORM,BIG,SMALL
   35 FORMAT(1H0,' GRADIENT NORM ',F10.4,2X,' AND CONDITION NUMBER',
     +E10.4,3X,E10.4)
      WRITE(6,4) FUN
    4 FORMAT(1H0,' FUNCTION VALUE = ',F12.6/)
      RETURN
      END
      SUBROUTINE BHHH(NPARAM,V,VMUS)
      LOGICAL IREC,LTHETA,JACOB
      LOGICAL DERIV,DERCUV,SUCCESS
      LOGICAL IFOK
      COMMON X(100,50)
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      COMMON /A8/ RES(20,20)
      COMMON /NAMES/ NAME(20)
      REAL NDERS,NDERJS
      EXTERNAL FUNML
      DIMENSION V(NPARAM),VMUS(NPARAM)
      DIMENSION SER(50),TRA(50)
      EE=1.E-10
      IMAX=300
      STEP=1.0
      TOL=1.E-3
      LTHETA=.FALSE.
      JACOB=.FALSE.
      MFUN=0
      MAXSQZ=10
      JSQZ=0
      SUCCESS=.FALSE.
      KPARAM=NPARAM+NQ
      IF(IMETH .GT. 0 .AND. ICOUNT .GT. 1) GO TO 999
C
C             DIFFERENTIATE W.R.T. ENDOGENOUS VARIABLES TO GET JACOBIAN
C
      CALL DIFIML(NPARAM,V)
      IF(NQ .GT. 10 .OR. KPARAM .GT. 50) GO TO 999
C
C             DIFFERENTIATE W,R.T. PARAMETERS
C
      DO 150 K1=1,NPARAM
      K=K1
      LTHETA=.TRUE.
      CALL DIFIML(NPARAM,V)
C
C             DIFFERENTIATE JACOBIAN W.R.T. PARAMETER
C
      JACOB=.TRUE.
      CALL DIFIML(NPARAM,V)
      JACOB=.FALSE.
  150 CONTINUE
C
C             EVALUATE ALL DERIVATIVES AND EQUATIONS AT EACH TIME PERIOD
C
  999 DO 1000 ITE=1,IMAX
```

```
      IF(IMETH .GT. 0) GO TO 158
      ICOUNT=ITE
      WRITE(6,1001) ITE
 1001 FORMAT(1HO,'ITERATION NUMBER ',I3)
      IF(ITE .GT. 1) GO TO 175
  158 CALL FUNML(NPARAM,V,FV)
      FUN=FV
      GO TO 176
  175 FUN=FUNNEW
  176 DO 170 K1=1,NPARAM
      SUM=0.
      DO 180 IT=1,NT
  180 SUM=SUM+VMU(IT,K1)
      VMUS(K1)=SUM
  170 CONTINUE
      IF(IMETH .GT. 0) RETURN
      WRITE(6,800)
  800 FORMAT(1HO,'GRADIENT VMUS')
      WRITE(6,801) (VMUS(J),J=1,NPARAM)
  801 FORMAT(1H ,8(E12.6,2X))
      VNORM=0.0
      DO 288 I=1,NPARAM
  288 VNORM=VNORM+VMUS(I)*VMUS(I)
      VNORM=SQRT(VNORM)
      WRITE(6,289) VNORM
  289 FORMAT(1HO,'GRADIENT NORM = ',F12.6)
      IF(VNORM .LE. 1.E-4) GO TO 1200
      IF(ITE .EQ. 1 .AND.NPARAM .LE. 10) CALL GCHECK(NPARAM,V,FUN,FUNML)
C
C            COMPUTE RIJ=VMU(PRIME)VMU
C
      DD=0.
      DO 195 I=1,NPARAM
      DO 190 J=1,NPARAM
      SUM=0.
      DO 185 M=1,NT
  185 SUM=SUM+VMU(M,I)*VMU(M,J)
      R(I,J)=SUM
  190 CONTINUE
  195 CONTINUE
      IF(NPARAM .GT. 10) GO TO 501
      WRITE(6,802)
  802 FORMAT(1HO,'HESSIAN MATRIX RIJ')
      DO 302 I=1,NPARAM
      WRITE(6,109) (R(I,J),J=1,I)
  109 FORMAT(1H ,8(E12.6,2X))
  302 CONTINUE
  501 CALL INVERT(R,NPARAM,DET)
      IF(NPARAM .GT. 10) GO TO 502
      WRITE(6,804)
  804 FORMAT(1HO,'RIJ (INVERSE)')
      DO 303 I=1,NPARAM
      WRITE(6,109) (R(I,J),J=1,I)
  303 CONTINUE
C
C            COMPUTE DIRECTION D
```

```
C
  502 DO 200 I=1,NPARAM
      SUM=0.
      DO 210 J=1,NPARAM
  210 SUM=SUM+R(I,J)*VMUS(J)
      D(I)=SUM
      DD=DD+D(I)*D(I)
  200 CONTINUE
      DD=SQRT(DD)
C
C            TEST FOR CONVERGENCE OF PARAMETER VECTOR THETA
C
      DO 270 I=1,NPARAM
      IF(ABS(D(I)) .GT. TOL*(ABS(V(I))+TOL*10.)) GO TO 600
  270 CONTINUE
      SUCCESS=.TRUE.
      IF(ISTEP .EQ. 1) GO TO 700
      GO TO 685
C
C            CONVERGENCE NOT ACHIEVED,DO LINEAR STEPSIZE SEARCH USING
C                          B+ALAMB*D VECTOR
  600 ALAMB=AMIN1(1.0,STEP/DD)
      DO 275 I=1,NPARAM
      TEMP(I)=V(I)
  275 CONTINUE
      GRAD=0.
      DO 280 I=1,NPARAM
      GRAD=GRAD+D(I)*VMUS(I)
  280 CONTINUE
      IF(ISTEP .EQ. 0) GO TO 680
      CALL BARD(FUN,FUNNEW,GRAD,ALAMB,MAXSQZ,IFOK,NSQZ,JSQZ,V,
     INPARAM,FUNML)
  700 WRITE(6,2000) FUN,FUNNEW,NSQZ,ALAMB,GRAD
 2000 FORMAT(' FUN=',F12.5,4X,' FUNNEW=',F12.5,4X,'NSQZ=',I4,'STEPSIZE='
     I,E12.5,4X,'GRAD=',E12.5)
      GO TO 690
  680 CALL GSTEP(FUN,FUNNEW,GRAD,ALAMB,NPARAM,V,FUNML,IFOK)
  685 WRITE(6,1999) FUN,FUNNEW,ALAMB,GRAD,MFUN
 1999 FORMAT(' FUN= ',F12.6,4X,' FUNNEW=',F12.6,4X,' STEPSIZE=',E12.6,
     +4X, ' GRAD=',E12.6,4X,' MFUN=',I4)
      DD=ALAMB*DD
      SN=AMAX1(STEP/2.0,2.0*DD)
      STEP=AMIN1(SN,2.0*STEP)
  690 WRITE(6,2001) (D(I),I=1,NPARAM)
 2001 FORMAT(' DIRECTION'/(8X,10E12.5))
      WRITE(6,2002) (V(I),I=1,NPARAM)
 2002 FORMAT(' PARAMETER ESTIMATES'/(8X,10E12.5))
      IF(SUCCESS )GO TO 1200
      IF(.NOT. IFOK) GO TO 1500
      IF(ISTEP .EQ. 0) GO TO 1000
      DO 710 I=1,NPARAM
  710 V(I)=TEMP(I)-ALAMB*D(I)
 1000 CONTINUE
      WRITE(6,2003) ITE
 2003 FORMAT(/' CONVERGENCE NOT ACHIEVED AFTER',I4,' ITERATIONS.'/)
      GO TO 1026
```

```
C
C          CONVERGENCE
C
 1200 WRITE(6,2004) ITE
 2004 FORMAT(' CONVERGENCE ACHIEVED AFTER',I4,' ITERATIONS.'/)
 1026 WRITE(6,2005) MFUN
 2005 FORMAT(' NUMBER OF FUNCTION EVALUATIONS =',I5/)
      IF(ITE .GT. 1) FUN=FUNNEW
      WRITE(6,2006) FUN
 2006 FORMAT(' LOG LIKELIHOOD FUNCTION = ',F15.7/)
C
C          COMPUTE STD-ERRORS AND T-RATIOS
C          OUTPUT STATISTICS
C
      DO 3080 J=1,NPARAM
      SER(J)=SQRT(R(J,J))
      IF(.NOT. IFOK) V(J)=TEMP(J)
      TRA(J)=V(J)/SER(J)
 3080 CONTINUE
      WRITE(6,3100)
 3100 FORMAT(1HO,5X,'PARAMETERS',10X,'STD-ERRORS',10X,'T-RATIOS')
      WRITE(6,3110)
 3110 FORMAT(1H ,5X,'----------',10X,'----------',10X,'--------'//)
      DO 3115 J=1,NPARAM
      WRITE(6,3120) NAME(J),V(J),SER(J),TRA(J)
 3120 FORMAT(1H ,A4,2X,F12.6,8X,F12.6,7X,F12.6)
 3115 CONTINUE
      WRITE(6,3225)
 3225 FORMAT(///'          RESIDUAL SUM OF SQUARES')
      WRITE(6,3226)
 3226 FORMAT(1H ,10X,'-----------------------'//)
      DO 3227 I=1,NB
      WRITE(6,3228) (RES(I,J),J=1,I)
 3228 FORMAT(1H ,5X,10F10.4)
 3227 CONTINUE
      WRITE(6,3311)
 3311 FORMAT(///'          VARIANCE-COVARIANCE MATRIX')
      WRITE(6,3312)
 3312 FORMAT(1H ,10X,'---------------------------'//)
      DO 3313 I=1,NPARAM
      WRITE(6,3314) (R(I,J),J=1,I)
 3314 FORMAT(1H ,10F12.6)
 3313 CONTINUE
      RETURN
C
C          FAILURE TO IMPROVE FUNCTION VALUE
C
 1500 WRITE(6,2007) ITE
 2007 FORMAT(/' FAILURE TO IMPROVE LIKELIHOOD FUNCTION AFTER',I4,'ITERAT
     1IONS.'/)
      GO TO 1026
      END
      SUBROUTINE BARD(FUN,FO,GRAD,RM,MAXSQZ,IFOK,NSQZ,JSQZ,V,NPARAM,
     IFUNCT)
      COMMON X(100,50)
      COMMON /A1/ NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),
     INADR(300),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      EXTERNAL FUNCT
      DIMENSION V(NPARAM)
      LOGICAL LTHETA,JACOB,IFOK
      IFOK=.TRUE.
      RMAX=1.E2
      KFLAG=0
      IFLAG=0
      NSQZ=0
      RO=1.0
    2 STEP=RO
      DO 140 J=1,NPARAM
  140 V(J)=TEMP(J)-STEP*D(J)
      CALL FUNCT(NPARAM,V,FV)
      IF(KFLAG .EQ. 1) GO TO 13
      IF(IFLAG .EQ. 1) GO TO 15
      FO=FV
      R1=-GRAD*RO**2/(2.*FO-2.*FUN-2.*GRAD*RO)
      WRITE(6,9000) GRAD,RO,FO,R1
 9000 FORMAT(' GRADIENT=',F12.7,' OLD STEPSIZE=',E15.7,' OLD F=',E15.7,
     I' NEW STEPSIZE=',E15.7)
      IF(FO .LT. FUN .AND. NSQZ .EQ. 0) GO TO 10
      IF(FO .LT. FUN) GO TO 13
      RO=AMAX1(.25*RO,AMIN1(.75*RO,R1))
      NSQZ=NSQZ+1
      JSQZ=JSQZ+1
      IF(NSQZ .LE. MAXSQZ) GO TO 2
      IFOK=.FALSE.
      RM=RO
      RETURN
   10 RR=RO
      R3=AMIN1(R1,.75*RMAX)
      IF(ABS(R3-RO) .LE. .1*RO .OR. R1 .LE. .25*RO) GO TO 11
      KFLAG=0
      RO=R3
      IFLAG=1
      GO TO 2
   15 F3=FV
      NSQZ=NSQZ+1
      JSQZ=JSQZ+1
      IF(F3 .LT. FO) GO TO 12
```

```
11 RO=RR
   IFLAG=0
   KFLAG=1
   GO TO 2
13 RM=RO
   FO=FV
   RETURN
12 RM=R3
   FO=F3
   RETURN
   END
```

```
      SUBROUTINE DIFIML(NPARAM,V)
      LOGICAL IREC,LTHETA,JACOB
      LOGICAL DERIV,DERCUV,SUCCESS
      COMMON X(100,50)
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      DIMENSION V(NPARAM)
      L=1
      NDIFF=0
      NNF=0
      ITAN=0
      LDIFF=0
      IF(.NOT. LTHETA) NTAN=0
      LFLAG=0
      IF(.NOT. LTHETA) NFLAG=0
C
C          JACOB IS TRUE FOR DIFFERENTIATING JACOBIAN W.R. T. PARAMETER
C          LTHETA IS TRUE FOR DIFFERENTIATING W.R.T. PARAMETER
C          LTHETA=FALSE FOR DIFFERENTIATING W.R.T. ENDOGENOUS VARIABLE
      IF(JACOB) GO TO 300
      NS=NQ
      IF(NINTF .NE. 0) NS=NQ+NINTF
      NJ=NS
      IF(NFLAG .EQ. 1 .AND. LTHETA) NS=NS+NTAN
      DO 185 I=1,NS
      IF(LTHETA .AND. NFLAG .EQ. 1 .AND. I .GT. NJ) GO TO 190
      IF(ICOUNT .GT. 1) GO TO 194
      NADMAX=LISTEN(I)
      WRITE(6,195) I,(NLIST(J),J=L,NADMAX)
  195 FORMAT(1HO,'EQUATION ',I4,/20I4)
  194 CALL PRIOR(NLIST,I,L,NPRIOR,NPRS,IREC,IFUNC,NDIFF,ICT)
      IF(LTHETA) GO TO 190
  198 IADC=NADR(IFUNC)+1
      DO 222 IDIFF=1,NDIFF
      DO 225 IVAL=1,NQ
      IF(LTHETA) GO TO 224
      IVAR=IVECT(NPARAM+IVAL)
  224 IADCD=MAXAD+1
      NFUNC=NFUNC+1
      MAXF=MAXF+1
      NPRIOR(MAXF)=NFUNC
      NPRS(NFUNC)=MAXF
      NDER(IFUNC,IVAR)=NFUNC+1000
      NADR(NFUNC)=IADCD
      CALL DIFF(IVAR,I)
      IF(LTHETA) GO TO 265
      IF(ITAN .EQ. 0) GO TO 250
      LFLAG=1
      IF(.NOT. LTHETA .AND. LFLAG .EQ. 1) NFLAG=LFLAG
      NPOINT=NPRS(NS)+NTAN
      NMOV=(MAXF-NPOINT)+NTAN
      JP=MAXF
      DO 246 JJ=1,NMOV
      NPT=NPRIOR(JP)
      NPRIOR(JP+1)=NPT
      JP=JP-1
      NPRS(NPT)=NPRS(NPT)+1
  246 CONTINUE
      MAXF=MAXF+1
      NPRIOR(JP+1)=NFUNC
      NPRS(NFUNC)=JP+1
      ITAN=0
  250 IADC=NADR(IFUNC)+1
  225 CONTINUE
  265 IF(.NOT. IREC) GO TO 270
      ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      IADC=NADR(IFUNC)+1
  222 CONTINUE
C
C             COMPLETE DIFFERENTIATING ALL RECURSIVE FUNCTIONS,
C             NOW RETURN TO DIFFERENTIATE FUNCTION I
C
      IREC=.FALSE.
      IFUNC=I
      GO TO 198
  190 IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 193
      IF(K .GT. 1) GO TO 196
      IF(I .GT. 1) GO TO 197
      LTMAXF=MAXF
      LTMAX=MAXAD
      LMAXF=NFUNC
      LTCONC=MAXCON
      GO TO 197
  196 IF(I .GT. 1) GO TO 197
      MAXAD=LTMAX
      MAXF=LTMAXF
      NFUNC=LMAXF
      MAXCON=LTCONC
      GO TO 197
  193 IF(I .GT. 1) GO TO 197
      LTFUNC(K)=NFUNC
  197 IVAR=IVECT(K)
      GO TO 198
  270 IF(LTHETA .AND. NFLAG .EQ. 1 .AND. I .GE. NJ) GO TO 271
      L=LISTEN(I)+1
      GO TO 272
  271 NNF=NNF+1
      IF(NNF .GT. NTAN) RETURN
      NPI=NPRS(NJ)
      IFUNC=NPRIOR(NPI+NNF)
      L=NADR(IFUNC)+1
      IREC=.FALSE.
      LDIFF=1
      NDIFF=1
      GO TO 273
  272 NDIFF=0
  273 NBB=NB
      IF(NINTF .NE. 0) NBB=NB+NINTF
      IF(NFLAG .EQ. 1) NBB=NBB+NTAN
      IF(LTHETA .AND. I .EQ. NBB) RETURN
  185 CONTINUE
      IF(.NOT. LTHETA) ICON(2)=MAXCON
      IF(LTHETA) ICON(3)=MAXCON
      RETURN
C
C          NOW DIFFERENTIATE JT W.R.T. THETA
C
  300 IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 301
      JTMAXF=NFUNC
      JMAXF=MAXF
      GO TO 302
  301 JFUNC(K)=NFUNC
C
C          GET DERIVATIVE FUNCTION AND ITS HEAD ADDRESS
C
  302 NDIFF=0
      KDIFF=0
      L=1
      IF(NFLAG .EQ. 1) NBB=NBB-NTAN
      DO 310 I=1,NBB
      KFLAG=0
      CALL PRIOR(NLIST,I,L,NPRIOR,NPRS,IREC,IFUNC,NDIFF,ICT)
      IF(IREC) KFLAG=1
      NPOINT=ICT
      KDIFF=NDIFF
      DO 320 J=1,NQ
      NDIFF=NDIFF+1
      DO 315 IDIFF=1,NDIFF
      IVAR=IVECT(NPARAM+J)
      KFUNC=NDER(IFUNC,IVAR)
      IF(KFUNC .LE. 1000) GO TO 325
      KFUNC=KFUNC-1000
      IADC=NADR(KFUNC)+1
      IADCD=MAXAD+1
      NFUNC=NFUNC+1
      MAXF=MAXF+1
      NPRIOR(MAXF)=NFUNC
      NPRS(NFUNC)=MAXF
      NADR(NFUNC)=IADCD
      IF(IREC) NDER(KFUNC,K)=NFUNC+1000
      IF(.NOT. IREC .AND. NFLAG .EQ. 1 .AND. I .LE. NINTF) NDER(KFUNC,K)
     +=NFUNC+1000
      IF(I .LE. NINTF) NDER(KFUNC,K)=NFUNC+1000
      NDERJ(IFUNC,J)=NFUNC+1000
      IF((NQ .LE. 10 .OR. KPARAM .LE. 50) .AND. IFUNC .EQ. I)
     +NDJ(I,K,J)=NFUNC+1000
      IVAR=IVECT(K)
      KVAR=J
      CALL DIFF(IVAR,I)
      IF(.NOT. IREC) GO TO 340
      GO TO 330
  325 IF(.NOT. IREC) GO TO 335
      IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 321
  330 NDERJ(IFUNC,J)=0
  321 ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      IF(IDIFF .EQ. KDIFF) IREC=.FALSE.
  315 CONTINUE
      GO TO 340
  335 IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 322
      NDERJ(IFUNC,J)=0
      GO TO 340
  322 NDJ(I,K,J)=0
  340 ICT=NPOINT
      NDIFF=KDIFF
      IFUNC=NPRIOR(ICT)
      IF(KFLAG .EQ. 1) IREC=.TRUE.
  320 CONTINUE
      L=LISTEN(I)+1
      NDIFF=0
      KDIFF=0
  310 CONTINUE
      ICON(4)=MAXCON
      RETURN
      END
      SUBROUTINE DIEVAL(NPARAM,V)
      LOGICAL IREC,LTHETA,JACOB
      LOGICAL DERIV,DERCUV,SUCCESS
      COMMON X(100,50)
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      DIMENSION V(NPARAM)
      DIMENSION VFLIST(200)
C
C
C            COMPUTE F AND F(PRIME)F
      DO 380 IT=1,NT
      L=1
      NDIFF=0
      NS=NB
      IF(NINTF .NE. 0) NS=NB+NINTF
      DO 400 I=1,NS
      CALL PRIOR(NLIST,I,L,NPRIOR,NPRS,IREC,IFUNC,NDIFF,ICT)
      VFUNC=0.
  410 IADC=NADR(IFUNC)+1
      IF(IREC) GO TO 420
      CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
      VFLIST(IFUNC)=VFUNC
      VLF(I,IT)=VFUNC
      GO TO 430
  420 DO 425 J=1,NDIFF
      CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
      VFLIST(IFUNC)=VFUNC
      VFUNC=0.
      ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      IADC=NADR(IFUNC)+1
  425 CONTINUE
      IREC=.FALSE.
      IFUNC=I
      GO TO 410
  430 L=LISTEN(I)+1
      NDIFF=0
  400 CONTINUE
C
C            NOW COMPUTE JT,GET FUNCTION AND ITS HEAD ADDRESS
C
      IF(NTAN .EQ. 0) GO TO 440
      VFUNC=0.
      ICT=NPRS(NS)+1
      DO 442 I=1,NTAN
      IFUNC=NPRIOR(ICT)
      IADC=NADR(IFUNC)+1
      CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
      VFLIST(IFUNC)=VFUNC
      VFUNC=0.
      ICT=ICT+1
  442 CONTINUE
  440 NS=NQ
      IF(NINTF .NE. 0) NS=NQ+NINTF
      ICT=NPRS(NS)
      IF(NTAN .GT. 0) ICT=ICT+NTAN
      IFUNC=NPRIOR(ICT+1)
      LTHETA=.FALSE.
      JACOB=.FALSE.
      IREC=.FALSE.
      DO 450 I=1,NS
  452 DO 455 J=1,NQ
      VFUNC=0.
      IVAR=IVECT(NPARAM+J)
      NFUNC=NDER(I,IVAR)
      IF(NFUNC .LE. 1000) GO TO 480
      NFUNC=NFUNC-1000
  460 IF(IFUNC .EQ. NFUNC) GO TO 465
      ICT=ICT+1
      IREC=.TRUE.
      IADC=NADR(IFUNC)+1
      GO TO 470
  465 IREC=.FALSE.
      IADC=NADR(IFUNC)+1
      ICT=ICT+1
  470 CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
      VFLIST(IFUNC)=VFUNC
      IF(IREC) GO TO 490
      VLF(IFUNC,IT)=VFUNC
      IFUNC=NPRIOR(ICT+1)
      GO TO 455
  490 IFUNC=NPRIOR(ICT+1)
      VFUNC=0.
      GO TO 460
  480 IF(NFUNC .EQ. 0) VFUNC=0.
      IF(NFUNC .EQ. 1) VFUNC=1.
      IF(NFUNC .EQ. -1) VFUNC=-1.
      IF(NFUNC .GT. 1) GO TO 485
      IF(NFUNC .LT. -1) GO TO 486
      GO TO 487
  485 VFUNC=CONS(NFUNC-1)
      GO TO 487
  486 VFUNC=-CONS(IABS(NFUNC)-1)
  487 NDERS(I,IVAR)=VFUNC
  455 CONTINUE
      IF(.NOT. IREC) GO TO 450
      IFUNC=NPRIOR(ICT+1)
      GO TO 452
  450 CONTINUE
      IF(IMETH .GT. 1 ) GO TO 380
C
C             EVALUATE PARTIAL D(FI)/D(THETA(K))
```

```
C           GET FUNCTION NUMBER AND ITS HEAD ADDRESS
C
      IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 505
      ICT=NPRS(LMAXF+1)
      GO TO 507
  505 ICT=NPRS(LTFUNC(K)+1)
  507 IFUNC=NPRIOR(ICT)
      LTHETA=.TRUE.
      JACOB=.FALSE.
      NS=NB
      IF(NINTF .NE. 0) NS=NB+NINTF
      DO 500 I=1,NS
      DERCUV=.FALSE.
      VFUNC=0.
      NFUNC=NDER(I,K)
      IVAR=K
      IF(NFUNC .LE. 1000) GO TO 526
      NFUNC=NFUNC-1000
  508 IF(IFUNC .EQ. NFUNC) GO TO 510
      IREC=.TRUE.
      IF(ICT .EQ. MAXF) GO TO 509
      IC=NPRIOR(ICT)
      ICN=NPRIOR(ICT+1)
      IF(IC .GT. ICN) GO TO 566
  509 IADC=NADR(IFUNC)+1
      GO TO 520
  566 IADC=NADR(IFUNC)+1
      DERCUV=.TRUE.
  510 IREC=.FALSE.
      IADC=NADR(IFUNC)+1
  520 CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
      IF(.NOT. DERCUV) GO TO 567
      VFLIST(IFUNC)=VFUNC
      VFUNC=0.
      ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      DERCUV=.FALSE.
      IADC=NADR(IFUNC)+1
      GO TO 520
  567 IF(IREC) GO TO 525
      VFLIST(IFUNC)=VFUNC
      VLF(IFUNC,IT)=VFUNC
      IF(ICT .GT. MAXF) GO TO 500
      ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      GO TO 500
  525 VFLIST(IFUNC)=VFUNC
      VFUNC=0.
      ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      IADC=NADR(IFUNC)+1
      GO TO 508
  526 IF(NFUNC .EQ. 0) VFUNC=0.
      IF(NFUNC .EQ. 1) VFUNC=1.
      IF(NFUNC .EQ. -1) VFUNC=-1.
      IF(NFUNC .GT. 1) GO TO 527
      IF(NFUNC .LT. -1) GO TO 528
      GO TO 530
  527 VFUNC=CONS(NFUNC-1)
      GO TO 530
  528 VFUNC=-CONS(IABS(NFUNC)-1)
  530 NDERS(I,IVAR)=VFUNC
  500 CONTINUE
      IF(NFLAG .EQ. 0) GO TO 544
      ICT=NPRS(NS)
      NS=NS+NTAN
      DO 540 I=1,NTAN
      VFUNC=0.
      ICT=ICT+1
      IFUNC=NPRIOR(ICT)
      NFUNC=NDER(IFUNC,K)
      IF(NFUNC .GT. 1000) GO TO 543
      GO TO 540
  543 NFUNC=NFUNC-1000
      IADC=NADR(NFUNC)+1
      CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)

      VFLIST(NFUNC)=VFUNC
  540 CONTINUE
  544 CONTINUE
C
C           NOW EVALUATE CROSS PARTIAL DERIVATIVE OF JT W.R.T. THETA
C           GET FUNCTION NUMBER AND ITS HEAD ADDRESS
C
      IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 545
      IF(JMAXF .EQ. MAXF) GO TO 551
      ICT=NPRS(JTMAXF+1)
      IFUNC=NPRIOR(ICT)
      GO TO 551
  545 IF(K .EQ. NPARAM) GO TO 553
      JF=LTFUNC(K)+1
      GO TO 554
  553 IF(NPRS(JFUNC(K)) .EQ. MAXF) GO TO 551
      JF=LTFUNC(K)+1
  554 IF(JF .EQ. JFUNC(K)) GO TO 551
      ICT=NPRS(JFUNC(K)+1)
      IFUNC=NPRIOR(ICT)
  551 LTHETA=.FALSE.
      JACOB=.TRUE.
      IF(NFLAG .EQ. 1) NS=NS-NTAN
      DO 550 I=1,NS
      IREC=.FALSE.
  552 DO 560 J=1,NQ
      VFUNC=0.
      IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 556
      NFUNC=NDERJ(I,J)
      GO TO 557
  556 NFUNC=NDJ(I,K,J)
  557 IF(NFUNC .LE. 1000) GO TO 580
      NFUNC=NFUNC-1000
  555 IF(IFUNC .EQ. NFUNC) GO TO 565
      IREC=.TRUE.
```

```
    IADC=NADR(IFUNC)+1
    GO TO 570
565 IREC=.FALSE.
    IADC=NADR(IFUNC)+1
570 CALL EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
    VFLIST(IFUNC)=VFUNC
    IF(IREC)GO TO 575
    VLF(IFUNC,IT)=VFUNC
    IF(ICT .EQ. MAXF) GO TO 560
    ICT=ICT+1
    IFUNC=NPRIOR(ICT)
    GO TO 560
575 ICT=ICT+1
    IFUNC=NPRIOR(ICT)
    VFUNC=0.
    GO TO 555
580 IF(NFUNC .EQ. 0) VFUNC=0.
    IF(NFUNC .EQ. 1) VFUNC=1.
    IF(NFUNC .EQ. -1) VFUNC=-1.
    IF(NFUNC .GT. 1) GO TO 582
    IF(NFUNC .LT. -1) GO TO 585
    GO TO 586
582 VFUNC=CONS(NFUNC-1)
    GO TO 586
585 VFUNC=-CONS(IABS(NFUNC)-1)
586 NDERJS(I,J)=VFUNC
560 CONTINUE
    IF(.NOT. IREC) GO TO 550
    IFUNC=NPRIOR(ICT+1)
    GO TO 552
550 CONTINUE
380 CONTINUE
    RETURN
    END
```

```
      SUBROUTINE PQEVAL(NPARAM,V)
      LOGICAL IREC,LTHETA,JACOB
      LOGICAL DERIV,DERCUV,SUCCESS
      COMMON X(100,50)
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      COMMON /A8/ RES(20,20)
      REAL NDERS,NDERJS
      DIMENSION V(NPARAM)
      DIMENSION F(100,20),S(50,50),H(50,50),DJ(50,50),PM(50,50)
      DIMENSION QM(50,50),G(50),DT(50)
      DETJT=0.
C
C            GET F,FORM F"F AND INVERT F"F
C
      DO 600 IT=1,NT
      IF(K .GT. 1) GO TO 618
      DO 610 I=1,NB
      IF(NINTF .EQ. 0) GO TO 605
      F(IT,I)=VLF(NINTF+I,IT)
      GO TO 610
  605 F(IT,I)=VLF(I,IT)
  610 CONTINUE
  600 CONTINUE
      CALL FPRIME(S,F,NB,NT)
      DO 801 I=1,NB
      DO 801 J=1,NB
      RES(I,J)=S(I,J)
  801 CONTINUE
      CALL INVERT(S,NB,DETF)
C
C            GET JT AND INVERT
C
  618 DO 615 IT=1,NT
      DO 620 I=1,NQ
      DO 630 J=1,NQ
      IVAR=IVECT(NPARAM+J)
      NFUNC=NDER(I,IVAR)
      IF(NINTF .NE. 0) NFUNC=NDER(NINTF+I,IVAR)
      IF(NFUNC .LE. 1000) GO TO 625
      NFUNC=NFUNC-1000
      H(I,J)=VLF(NFUNC,IT)
      GO TO 630
  625 H(I,J)=NDERS(I,IVAR)
      IF(NINTF .NE. 0) H(I,J)=NDERS(NINTF+I,IVAR)
  630 CONTINUE
  620 CONTINUE
      CALL INVERT(H,NB,DETJ)
      DET=ALOG(ABS(DETJ))
      DETJT=DETJT+DET
      IF(IMETH .GT. 1 ) GO TO 615
C
C           GET PARTIAL D(J(IJ))/D(THETA(K)) MATRIX
C
      DO 640 I=1,NB
      DO 650 J=1,NQ
      IF(NQ .LE. 10 .OR. KPARAM .LE. 50) GO TO 643
      NFUNC=NDERJ(I,J)
      IF(NINTF .NE. 0) NFUNC=NDERJ(NINTF+I,J)
      GO TO 644
  643 NFUNC=NDJ(I,K,J)
      IF(NINTF .NE. 0) NFUNC=NDJ(NINTF+I,K,J)
  644 IF(NFUNC .LE. 1000) GO TO 645
      NFUNC=NFUNC-1000
      DJ(I,J)=VLF(NFUNC,IT)
      GO TO 650
  645 DJ(I,J)=NDERJS(I,J)
      IF(NINTF .NE. 0) DJ(I,J)=NDERJS(NINTF+I,J)
  650 CONTINUE
  640 CONTINUE
C          COMPUTE P
      DO 660 I=1,NB
      DO 670 J=1,NB
      PSUM=0.
      DO 680 M=1,NB
  680 PSUM=PSUM+H(I,M)*DJ(M,J)
      PM(I,J)=PSUM
  670 CONTINUE
  660 CONTINUE
      P=0.
      DO 690 I=1,NB
      DO 690 J=1,NB
      IF(I .NE. J) GO TO 690
      P=P+PM(I,J)
  690 CONTINUE
C
C           COMPUTE G(IT)=F"F(INVERSE)*F"(T)
C
      DO 700 I=1,NB
      PSUM=0.
      DO 710 J=1,NB
  710 PSUM=PSUM+S(I,J)*F(IT,J)
      G(I)=PSUM
  700 CONTINUE
C
C           GET PARTIAL D(FI)/D(THETA K) VECTOR
C
      DO 720 I=1,NB
      NFUNC=NDER(I,K)
      IF(NINTF .NE. 0) NFUNC=NDER(NINTF+I,K)
      IF(NFUNC .LE. 1000) GO TO 715
      NFUNC=NFUNC-1000
      DT(I)=VLF(NFUNC,IT)
      GO TO 720
  715 DT(I)=NDERS(I,K)
      IF(NINTF .NE. 0) DT(I)=NDERS(NINTF+I,K)
  720 CONTINUE
C
C           COMPUTE Q
C
      Q=0.
      DO 730 I=1,NB
      Q=Q+DT(I)*G(I)
  730 CONTINUE
C           STORE (P-Q)
      VMU(IT,K)=Q-P
  615 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE FPRIME(S,F,NB,NT)
      DIMENSION S(50,50),F(100,20)
      DO 220 I=1,NB
      DO 225 J=1,NB
      SUM=0.
      DO 230 M=1,NT
  230 SUM=SUM+F(M,I)*F(M,J)
      S(I,J)=SUM/FLOAT(NT)
  225 CONTINUE
  220 CONTINUE
      RETURN
      END
      SUBROUTINE PRIOR(NLIST,I,L,NPRIOR,NPRS,IREC,IFUNC,NDIFF,ICT)
      LOGICAL IREC
      DIMENSION NLIST(4000),NPRIOR(300),NPRS(300)
C
C            THIS SUBROUTINE IS TO CHECK PRIORITY ORDERING OF FUNCTIONS
C            FUNCTION IN INNER BRACKET IS ALLOCATED WITH HIGHER PRIORITY
C            THAN FUNCTION IN OUTER BRACKET
      IC=NLIST(L)
      ICT=NPRS(IC)
      IF(ICT .EQ. I) GO TO 210
      IC=ICT
      NPOINT=ICT
      IREC=.TRUE.
  200 ICT=ICT-1
      IF(ICT .EQ. 0) GO TO 220
      IPR=NPRIOR(ICT)
      IF(IPR .LT. I) GO TO 220
      IR=NPRS(IPR)
      IF(IR-IC) 205,201,201
  201 WRITE(6,202) IC
  202 FORMAT(1HO,'FUNCTION',I3,' HAS THE WRONG PRIORITY')
      RETURN
  205 IC=IR
      GO TO 200
  210 IREC=.FALSE.
      IFUNC=I
      RETURN
  215 IREC=.FALSE.
      NDIFF=1
      IFUNC=NPRIOR(ICT)
      RETURN
  220 ICT=ICT+1
      IF(ICT .EQ. NPOINT) GO TO 215
      NDIFF=NPOINT-ICT
      IFUNC=NPRIOR(ICT)
      RETURN
      END
      SUBROUTINE INVERT(A,N,D)
      DIMENSION A(50,50),L(50),M(50)
C          THE INVERSE OF THE MATRIX IS CALCULATED USING GAUSS JORDAN
C          WITH COMPLATE PIVOTING.THE INVERSE REPLACES THE ORIGINAL
C          MATRIX.L AND M ARE WORK VECTORS OF LENGTH N.THE DETERMINANT
C          D IS CALCULATED
C
      D=1.0
      DO 190 K=1,N
      L(K)=K
      M(K)=K
      BIG=A(K,K)
      DO 20 I=K,N
      DO 20 J=K,N
      IF(ABS(BIG)-ABS(A(I,J))) 10,20,20
   10 BIG=A(I,J)
      L(K)=I
      M(K)=J
   20 CONTINUE
C          CHECK FOR SINGULARITY
      IF(BIG) 40,30,40
   30 D=0.0
      RETURN
C          INTERCHANGE ROWS
   40 I=L(K)
      IF(I-K) 50,70,50
   50 DO 60 J=1,N
      TEMP=-A(K,J)
      A(K,J)=A(I,J)
   60 A(I,J)=TEMP
C          INTERCHANGE COLUMNS
   70 J=M(K)
      IF(J-K) 80,100,80
   80 DO 90 I=1,N
      TEMP=-A(I,K)
      A(I,K)=A(I,J)
   90 A(I,J)=TEMP
C          DIVIDE COLUMN BY MINUS PIVOT
  100 DO 120 I=1,N
      IF(I-K) 110,120,110
  110 A(I,K)=A(I,K)/(-BIG)
  120 CONTINUE
C          REDUCE MATRIX
      DO 160 I=1,N
      IF(I-K) 130 ,160,130
  130 TEMP=A(I,K)
      DO 150 J=1,N
      IF(J-K) 140,150,140
  140 A(I,J)=TEMP*A(K,J)+A(I,J)
  150 CONTINUE
  160 CONTINUE
C          DIVIDE ROW BY PIVOT
      DO 180 J=1,N
      IF(J-K) 170,180,170
  170 A(K,J)=A(K,J)/BIG
  180 CONTINUE
```

```
C           CALCULATE DETERMINANT
      D=D*BIG
C           TAKE RECIPROCAL
  190 A(K,K)=1.0/BIG
C           BACK SUBSTITUTION
      NM1=N-1
      IF(NM1) 200,270,200
  200 DO 260 KK=1,NM1
      K=N-KK
      J=L(K)
      IF(J-K) 210,230,210
  210 DO 220 I=1,N
      TEMP=A(I,K)
      A(I,K)=-A(I,J)
  220 A(I,J)=TEMP
  230 I=M(K)
      IF(I-K) 240,260,240
  240 DO 250 J=1,N
      TEMP=A(K,J)
      A(K,J)=-A(I,J)
  250 A(I,J)=TEMP
  260 CONTINUE
  270 RETURN
      END
```

```
      SUBROUTINE RDCARD(ITEXT)
      DIMENSION ITEXT(80)
      READ(5,1000) (ITEXT(I),I=1,80)
 1000 FORMAT(80A1)
      WRITE(6,1001) (ITEXT(I),I=1,80)
 1001 FORMAT(1H0,2X,40A1/1H0,2X,40A1)
      RETURN
      END
      SUBROUTINE FRML(ITEXT,NFUNC,N,IADC,IEND,MAXCON,MAXF,KC,ISYM)
C
C          FORMULA PROCESSOR
C
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      DIMENSION IREPS(20),NANTS(20),NTERS(20),NANFS(20),NFACS(20)
      DIMENSION LSYM(33),ITEXT(80)
      DIMENSION ISYM(200)
      LOGICAL IEND
      DATA LSYM/1HV,1HF,1H*,1H/,1H+,1H-,1HO,1H1,1H2,1H3,1H4,1H5,1H6,
     I1H7,1H8,1H9,1H.,1H),1H=,1HL,1HE,1HS,1HC,1HA,1HN,1HG,1HX,1HP,
     I1HI,1HO,1HR,1HT,1H(/
      DATA JBLANK/1H /
      DATA JD/1H$/
C
C          INITIALIZATION
C
      IEND= .FALSE.
      JCOUNT=0
      NDEPTH=0
      NSYM=0
      ISIGN=1
      IREP=0
      ISET=0
      ISPEC=0
      K=0
    1 ICOUNT=0
C
C          INPUT FORMULA WITH SYMBOLS
C          COUNT NUMBER OF SYMBOLS AND PUT ADDRESS OF EACH
C          SYMBOL IN NLIST
C          NSYM IS NUMBER OF SYMBOLS IN EACH EXPRESSION
C          ICOUNT TESTS END OF EACH FUNCTION DEFINITION
C          JCOUNT IS TERMINATOR OF INPUT
C
    2 DO 10 I=1,80
      JX=ITEXT(I)
      DO 12 J=1,33
      IF(JX .NE. LSYM(J)) GO TO 12
      ICOUNT=0
      K=K+1
      GO TO 15
   12 CONTINUE
      IF(JX .EQ. JBLANK) GO TO 13
      IF(JX .EQ. JD) GO TO 18
      WRITE(6,9) JX,I
    9 FORMAT(1HO,'ILLEGAL CHARACTER ',A1,'FOUNT AT SYMBOL',I3)
      RETURN
   15 ISYM(K)=J
      NSYM=NSYM+1
      GO TO 14
   13 ICOUNT=ICOUNT+1
   14 IF(ICOUNT .GE. 3) GO TO 16
      GO TO 10
   18 JCOUNT=JCOUNT+1
```

```
      IF(JCOUNT .NE. 4) GO TO 10
      IEND=.TRUE.
      RETURN
   10 CONTINUE
      IF(ICOUNT .GE. 3) GO TO 16
      CALL RDCARD(ITEXT)
      GO TO 2
   16 ISYM(NSYM+1) =18
C
C             INITIALIZE NUMBER ROUTINE TO GET INDEX OF FUNCTION VARIABLE,
C             POWER OR CONSTANT
C             ISWIT =1 AND 2 INTEGER,3 AND 4 REAL NUMBER
C             IDEC =0 AFTER  "." AND INCREASE BY  ONE TO COUNT NUMBER
C             OF DECIMAL PLACES
C             ID IS THE NEXT INTEGER IN THE SYMBOL LIST
C
      ILIST=1
      IC=ISYM(ILIST)
      IF(IC .NE. 2) GO TO 100
      ISWIT=1
      IDEC=-1
      IC=1
      ILIST=2
      NUM=0
      CALL NUMBER(ISYM,IC,N,ILIST,IDEC,ISWIT,NUM,CONS,MAXCON,ID,IREP,
     ICONC,NFNUM)
      GO TO (27,41,56,32),ISWIT
   27 NLIST(IADC)=NUM
      NFNUM=NUM
      NADR(NFNUM)=IADC
      MAXF=MAXF+1
      NPRIOR(MAXF)=NFNUM
      NPRS(NFNUM)=MAXF
C             NFACT=-1 SHOWS CONSTANT HAS NOT  YET READ
      NADNT=IADC+1
      NADNF=NADNT+1
      IADC=NADNF+2
      NFACT=-1
      NTERM=1
C             SYMBOL IS "=",SKIP TO NEXT INTEGER IN ISYM
      IF(ID .NE. 12) GO TO 100
   28 ILIST=ILIST+1
      IC=ISYM(ILIST)
C             ")" NOT ALLOWED
C             TEST FOR "-"
C
      IF(IC .EQ. 18) GO TO 100
      IF(IC .NE. 6) GO TO 31
   29 ISIGN=-1
   30 ILIST=ILIST+1
      IC=ISYM(ILIST)
C             IF TEST IS TRUE EXPECTS "V" OR "F"
   31 IF(IC .LE. 6) GO TO 40
      ID=IC-7
C             IF TEST IS TRUE EXPECTS SPECIAL FUNCTIONS
      IF(ID .GE. 11) GO TO 45
```

```
C          START PROCESSING CONSTANT
      ISWIT=4
      IC=ILIST
      NUM=0
      IDEC=-1
      IF(ID .LT. 10) GO TO 21
      IDEC=0
   22 CALL NUMBER(ISYM,IC,N,ILIST,IDEC,ISWIT,NUM,CONS,MAXCON,ID,IREP,
     ICONC,NFNUM)
      GO TO 32
   21 NUM=10*NUM+ID
      GO TO 22
   32 IF(NFACT .EQ. -1) GO TO 34
      IC=NLIST(NADNF+1)
      IF(IC .GT. 0) GO TO 33
      ISIGN=-ISIGN
      IC=-IC
   33 IC=IC-1
      IF(IC .GT. 0) GO TO 35
   34 IDT=MAXCON+1
      IF(ISIGN .LT. 0) IDT=-IDT
      NLIST(NADNF+1)=IDT
      IF(NFACT .EQ. -1) NFACT=0
      ISPEC=0
      GO TO 37
   35 CONS(IC)=CONC*CONS(IC)
      MAXCON=MAXCON-1
      IC=IC+1
      IF(ISIGN .LT. 0) IC=-IC
      NLIST(NADNF+1)=IC
   37 ISIGN=1
      IF(ID .EQ. 11) GO TO 75
      IF(ID .EQ. 12) GO TO 100
C
C          IF TEST IS TRUE,EXPECTS "+" OR "-"
C          ELSE IF ID=-3 THEN EXPECTS "/"
      IF(ID .GT. -3) GO TO 39
      IF(ID .NE. -3) GO TO 38
      IREP=-15
      GO TO 28
   38 IF(ID .LT. -4) GO TO 100
C
C          TEST FOR "**"
      IF(ISYM(ILIST+1) .EQ. 3) GO TO 55
      IREP=0
      GO TO 28
C
C          COMPLETES DESCRIPTION OF PREVIOUS TERM
C          SET UP PARAMETERS FOR NEXT TERM
C

   39 NLIST(NADNF)=NFACT
      IREP=0
      NADNF=IADC
      NTERM=NTERM+1
      IADC=NADNF+2
      NFACT=-1
```

```
C
C          ID=-1 EXPECTS "-"
C          ID=-2 EXPECTS "+"
C
      IF(ID .EQ. -1) GO TO 29
      GO TO 30
C          SECTION FOR "V" AND "F"
   40 IF(IC .GT. 2) GO TO 100
      IF(NFACT .GE. 0) GO TO 42
      NLIST(IADC-1)=ISIGN
      ISIGN=1
      NFACT=0
   42 NFACT=NFACT+1
      IF(ISIGN .LT. 0) GO TO 100
      ISPEC=0
C          SET UP NUMBER ROUTINE FOR V OR F
C          STORE V OR F IN APPROPRIATE ADDRESS OF NLIST
C
      IDEC=-1
      IFC=IC
      IC=ILIST
      ILIST=ILIST+1
      NUM=0
      ISWIT=2
      CALL NUMBER(ISYM,IC,N,ILIST,IDEC,ISWIT,NUM,CONS,MAXCON,ID,IREP,
     ICONC,NFNUM)
   41 NUM=NUM+5
      IF(IFC .EQ. 2) NUM=NUM+995
      NLIST(IADC)=NUM
      IADC=IADC+1
      IF(IREP .EQ. 0) GO TO 37
      NLIST(IADC)=-15
      IADC=IADC+1
      GO TO 37
C
C          SECTION FOR SPECIAL FUNCTIONS
C                 1 = LOG
C                 2 = EXP
C                 3 = SIN
C                 4 = COS
C                 5 = ARCTAN
C
   45 IF(NFACT .GE. 0) GO TO 44
      NLIST(IADC-1)=ISIGN
      ISIGN=1
      NFACT=0
C          IF TEST IS TRUE,EXPECTS "("
   44 IF(ID .EQ. 26) GO TO 70
      IF(ID .GE. 19) GO TO 100
      IF(ISPEC .EQ. 1) GO TO 100
      ISPEC=1
      IDD=ID-12
      GO TO (46,47,48,49,50,51),IDD
C          TEST FOR "LOG"
   46 ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 30) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 26)GO TO 100
      NLIST(IADC)=1
      IADC=IADC+1
      GO TO 30
C          TEST FOR  "EXP"
   47 ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 27) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 28) GO TO 100
      NLIST(IADC)=2
      IADC=IADC+1
      GO TO 30
C          TEST FOR "SIN"
   48 ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 29) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 25) GO TO 100
      NLIST(IADC)=3
      IADC=IADC+1
      GO TO 30
C          TEST FOR "COS"
   49 ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 30) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 22) GO TO 100
      NLIST(IADC)=4
      IADC=IADC+1
      GO TO 30
C          TEST FOR "ARCT" FOR ARCTANGENT
   50 ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 32) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 24) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 25) GO TO 100
      NLIST(IADC)=5
      IADC=IADC+1
      GO TO 30
C
C          SECTION FOR KEY WORD "NEXT"
C
   51 ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 21) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 27) GO TO 100
      ILIST=ILIST+1
      IF(ISYM(ILIST) .NE. 32) GO TO 100
      CALL RDCARD(ITEXT)
      GO TO 1
C
C          SECTION FOR "**"
C
   55 NUM=0
      ISWIT=3
      IC=ILIST+1
      ILIST=IC+1
      ISET=IREP
      ID=ISYM(ILIST)-7
      IF(ID .NE. -1) GO TO 54
      IREP=IREP-15
      IC=ILIST
      ILIST=ILIST+1
   54 CALL NUMBER(ISYM,IC,N,ILIST,IDEC,ISWIT,NUM,CONS,MAXCON,ID,IREP,
     ICONC,NFNUM)
   56 IF(IDEC .GT. 0) GO TO 57
C             IF PREVIOUS OPERATOR WAS "/" THEN INSERT "**-1"
      IF(IREP .EQ. 0) GO TO 58
      IF(IREP .EQ. -15) NUM=-NUM
      IREP=0
      IF(ISET .EQ. -15) IADC=IADC-1
   58 IF(NUM .GT. 10) GO TO 57
      IF(NUM .LT. -15) GO TO 57
      NUM=-NUM-16
      GO TO 59
   57 IF(IREP .EQ. 0) GO TO 60
      IF(ISET .EQ. -15) IADC=IADC-1
      IF(IREP .LT. -15) CONC=-CONC
      IREP=0
      CONS(MAXCON)=-CONC
   60 NUM=-26-MAXCON
   59 NLIST(IADC)=NUM
      IADC=IADC+1
      GO TO 37
C
C             SECTION FOR "(",EXPECTS NEW FUNCTION AND UNCONDITIONAL JUMP
C             INCREASE DEPTH OF NESTED FUNCTION
C             STORE PARAMETERS FOR OUTER FUNCTION
C
   70 IADC=IADC+1
      NLIST(IADC)=-16
      KC=KC+1
      JUMPAD(N,KC)=IADC
      IADC=IADC+2
      NDEPTH=NDEPTH+1
      IREPS(NDEPTH)=IREP
      NANTS(NDEPTH)=NADNT
      NFACT=NFACT+1
      NFACS(NDEPTH)=NFACT
      NTERS(NDEPTH)=NTERM
      NANFS(NDEPTH)=NADNF
      MAXF=MAXF+1
      NFUNC=NFUNC+1
      NLIST(IADC-3)=NFUNC+1000
      NLIST(IADC)=NFUNC
      NADR(NFUNC)=IADC
C             SET UP PRIORITY ORDERING AND REVERSE ORDERING OF FUNCTIONS
      IC=NLIST(NADNT-1)
      ICT=NPRS(IC)
      NMOV=MAXF-ICT
      ICT=MAXF
      DO 71 IC=1,NMOV
      NPT=NPRIOR(ICT-1)
      NPRIOR(ICT)=NPT
      ICT=ICT-1
      NPRS(NPT)=NPRS(NPT)+1
   71 CONTINUE
      NPRIOR(ICT)=NFUNC
      NPRS(NFUNC)=ICT
C          SET UP PARAMETERS FOR INNER FUNCTION
      NADNT=IADC+1
      NADNF=NADNT+1
      IADC=NADNF+2
      IREP=0
      NFACT=-1
      NTERM=1
      GO TO 28
C
C          SECTION FOR ")"
C
   75 IF(ILIST .GT. NSYM) GO TO 91
      IF(NDEPTH .GT. 0) GO TO 76
   74 WRITE(6,150) NFNUM,ILIST
  150 FORMAT(1H0,'DEFINITION OF FUNCTION',I3,'HAS A SURPLUS RIGHT BRACKE
     1T AT SYMBOL',I3)
      ILIST=ILIST+1
      ID=ISYM(ILIST)-7
      GO TO 37
C
C          PUT ADDRESS FOR JUMP FROM OPENING BRACKER
C          CLEAR UP END OF INNER FUNCTION
C          RESET VALUES FOR OUTER FUNCTION
C
   76 IC=NADNT-2
      NLIST(IC)=IADC
      NLIST(NADNT)=NTERM
      NLIST(NADNF)=NFACT
      NTERM=NTERS(NDEPTH)
      NADNT=NANTS(NDEPTH)
      NFACT=NFACS(NDEPTH)
      NADNF=NANFS(NDEPTH)
      IREP=IREPS(NDEPTH)
      NDEPTH=NDEPTH-1
C          TEST WHETHER BRACKETS ARE UNNECESSARY
      ID=IADC-IC
      IF(ID .GT. 6) GO TO 78
      IF(ID .LT. 6) RETURN
      ID=NLIST(IC-2)
      IF(ID .NE. 1) GO TO 78
      NLIST(IC-2)=NLIST(IADC-1)
      IADC=IC-1
      ILIST=ILIST+1
      ID=ISYM(ILIST)-7
      GO TO 37
C          JUMP IS UNNECESSARY BECAUSE OUTER AND INNER FUNCTIONS
C          END TOGETHER
   78 ILIST=ILIST+1
      ID=ISYM(ILIST)-7
      IF(ID .EQ. 11) GO TO 72
      IF(IREP .EQ. 0) GO TO 37
      NLIST(IADC)=-15
      IADC=IADC+1
      IREP=0
      GO TO 37
   72 IF(ILIST .GT. NSYM) GO TO 73
      IF(NDEPTH .EQ. 0) GO TO 74
   73 NLIST(IC-1)=IREP
      NLIST(IC)=0
      IREP=0
      DO 82 JZ=1,KC
      IF(JUMPAD(N,JZ) .EQ. IC-1) JUMPAD(N,JZ)=0
   82 CONTINUE
      GO TO 75
C          END OF FUNCTION SPECIFICATION
   91 NLIST(NADNT)=NTERM
      NLIST(NADNF)=NFACT
      IF(NDEPTH .EQ. 0) RETURN
      WRITE(6,94) NFNUM
   94 FORMAT(1HO,'DEFINITION OF FUNCTION',I3,'HAS TOO FEW LEFT HAND BRAC
     1KETS')
      IC=NADNT-3
      NLIST(IC)=IREPS(NDEPTH)
      NLIST(IC+1)=0
      NTERM=NTERS(NDEPTH)
      NFACT=NFACS(NDEPTH)
      NADNT=NANTS(NDEPTH)
      NADNF=NANFS(NDEPTH)
      NDEPTH=NDEPTH-1
      GO TO 91
  100 WRITE(6,101) NFNUM,ILIST
  101 FORMAT(1HO,'ERROR IN THE DEFINITION OF FUNCTION',I3,'AT SYMBOL',
     1I3,'SHOULD NOT OCCUR')
      RETURN
      END
      SUBROUTINE NUMBER(ISYM,IC,N,ILIST,IDEC,ISWIT,NUM,CONS,MAXCON,ID,
     IIREP,CONC,NFNUM)
      DIMENSION CONS(200),ISYM(200)
   19 IC=IC+1
      ID=ISYM(IC)-7
C
C          ID NEGATIVE INDICATES END OF NUMBERS
C          ID GREATER THAN 10 INDICATES ")" OR "=" FOLLOWS NUMBER
C
      IF( ID .LT. 0) GO TO 23
      IF(ID .GT. 12) GO TO 100
      IF(ID .GT. 10) GO TO 23
      IF(IDEC .GE. 0) GO TO 20
      IF(ID .LT. 10) GO TO 21
      IDEC=0
      GO TO 19
   20 IDEC=IDEC+1
   21 NUM=10*NUM+ID
      GO TO 19
   23 IF(ILIST .EQ. IC) GO TO 100
      ILIST=IC
      IF(ISWIT .GT. 2) GO TO 24
      IF(IDEC .GT. 0) GO TO 102
      RETURN
   24 CONC=FLOAT(NUM)
      IF(ISWIT .EQ. 3 .AND. IDEC .LE. 0) RETURN
      IF(IDEC .LE. 0) GO TO 26
      SCALE=1.
      DO 25 I=1,IDEC
   25 SCALE=10.*SCALE
      CONC=CONC/SCALE
   26 IC=ISWIT+IREP
      IF(IC .NE. -11) GO TO 17
      IREP=0
      CONC=1.0/CONC
   17 MAXCON=MAXCON+1
      CONS(MAXCON)=CONC
      RETURN
  100 WRITE(6,101) NFNUM,ILIST
  101 FORMAT(1HO,'ERROR IN THE DEFINITION OF FUNCTION',I3,'AT SYMBOL',
     II3,'SHOULD NOT OCCUR')
      RETURN
  102 WRITE(6,103) NFNUM,ILIST
  103 FORMAT(1HO,'DECIMAL POINT IN THE DEFINITION FUNCTION' I3,'AT SYMBO
     IL',I3,'SHOULD NOT OCCUR')
      RETURN
      END
      SUBROUTINE DIFF(IVAR,I)
C
C          DIFFERENTIATION SUBROUTINE
C
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      LOGICAL JACOB
      LOGICAL IREC
      LOGICAL SKIP
      LOGICAL LJUMP
      LOGICAL LTHETA
      NTERMD=0
      NLIST(IADCD)=NFUNC
      L=IADCD
      IADCD=IADCD+2
      NTERM=NLIST(IADC)
      IADC=IADC+1
C
C          DIFFERENTIATE TERM BY TERM
C          ICLIST IS CONSTANT IN CURRENT TERM
C          ITRAN GIVES START OF DESCRIPTION OF FACTER IN CURRENT TERM
C
      DO 100 I1=1,NTERM
      SKIP=.TRUE.
      NFACT=NLIST(IADC)
      IADC=IADC+1
      IF(NFACT .EQ. 0) GO TO 96
      ICLIST=NLIST(IADC)
      ITRAN=IADC+1
      GO TO 95
   96 IADC=IADC+1
      GO TO 100
C
C          DIFFERENTIATE USING PRODUCT FORMULAE
C          WITH ONE TERM FOR EACH FACTOR
C
   95 DO 97 J=1,NFACT
      LJUMP=.FALSE.
      IADC=IADC+1
      ICOP=IADC
      ID=NLIST(IADC)
      IF(ID .GT. 5) GO TO 1
      IADC=IADC+1
      ID1=NLIST(IADC)
      IDNT=1
      GO TO 2
    1 ID1=ID
      IDNT=0
```

```
C             ID2 IS USED TO TEST FOR EXPONENT
    2 ID2=NLIST(IADC+1)
      IF(ID2 .GE. 0) GO TO 3
      IADC=IADC+1
      IF(ID2 .EQ. -16) GO TO 8
      IF(LDIFF .EQ. 1) GO TO 3
      IPWR=IADC
      IF(JC(I) .EQ. 0) GO TO 3
      KK=JC(I)
      IF((KK .EQ. 1) .AND. (JUMPAD(I,KK) .EQ. 0)) GO TO 3
      DO 93 JK=1,KK
      KC=JUMPAD(I,JK)
      IF(KC .EQ. 0) GO TO 93
      KC=NLIST(KC+1)
      IF(KC .EQ. IPWR) GO TO 99
   93 CONTINUE
      GO TO 3
   99 IF(LJUMP) GO TO 3
      ID2=0
    3 IF(ID1 .GT. 1000) GO TO 4
      IDNT=IDNT-1
      IC=ID1-IVAR
      IF(IC .NE. 5) GO TO 97
      GO TO 40
    4 IF(NDER(ID1-1000,IVAR) .EQ. 0) GO TO 97
      GO TO 40
   40 SKIP=.FALSE.
      IFACC=IADCD
      IADCD=IFACC+1
      NLIST(IADCD)=ICLIST
      IADCD=IADCD+1
      IFACT=0
      IF(J .EQ. 1) GO TO 9
      ICC=ITRAN
      ISWIT=0
      IFLAG=0
C
C             TRANSFER INITIAL AND FINAL NON-DIFFERENTIATED FACTORS
C             TO THE DERIVATIVE
C             OMITS JUMPS FROM THE DERIVATIVE
C
    7 IC=NLIST(ICC)
      IF(IC .GT. 5) IFACT=IFACT+1
      ICC=ICC+1
      IF(IFLAG .EQ. 1) GO TO 73
      IF(ISWIT .NE. 0 .AND. NLIST(ICC) .LT. 0) ICOP=ICOP+1
      IF(ISWIT .NE. 0 .AND. IC .GT. 0 .AND. IC .LE. 5) ICOP=ICOP+1
      IF(ISWIT .NE. 0 .AND. NLIST(ICC) .EQ. -16) ICOP=NLIST(ICOP)+1
   73 IF(IC .NE. -16) GO TO 5
      ICC=NLIST(ICC)
      GO TO 6
    8 LJUMP=.TRUE.
      IADC=NLIST(IADC+1)-1
      GO TO 2
    5 NLIST(IADCD)=IC
      IADCD=IADCD+1
    6 IF(IFLAG .EQ. 1) GO TO 74
      IF(ICC .NE. ICOP) GO TO 7
   74 IF(ISWIT .EQ. 1) GO TO 43
      GO TO 44
   43 IFLAG=1
      IF(IFACT .LT. NFACT) GO TO 7
   44 IF(ISWIT .EQ. 1) GO TO 31
    9 IF(ID .GT. 5) GO TO 16
      GO TO (10,11,12,13,14),ID
C             DERIVATIVE HAS THE FORM X**-1 OR F**-1
   10 NLIST(IADCD)=ID1
      IADCD=IADCD+1
      NLIST(IADCD)=-15
      IADCD=IADCD+1
      GO TO 16
C
C             DERIVATIVE HAS THE FORM EXP(X) OR EXP(F)
   11 NLIST(IADCD)=2
      GO TO 15
C
C             DERIVATIVE HAS THE FORM COS(X) OR COS(F)
C
   12 NLIST(IADCD)=4
      GO TO 15
C
C             DERIVATIVE HAS THE FORM -SIN(X) OR -SIN(F)
C
   13 NLIST(IADCD)=3
      ICLIST=-ICLIST
      IF(ICLIST .EQ. 0) ICLIST=-1
      NLIST(IFACC+1)=ICLIST
      GO TO 15
C
C             FOR ARCTAN DEFINE A NEW FUNCTION AS 1+X**2 OF 1+F**2
C             INVERT THE FUNCTION
C
   14 NFUNC=NFUNC+1
      IF(LTHETA .OR. JACOB)MAXF=MAXF+1
      NLIST(IADCD)=NFUNC+1000
      NADR(NFUNC)=IADCD
      IADCD=IADCD+1
      NLIST(IADCD)=-16
      IADCD=IADCD+1
      NLIST(IADCD)=IADCD+9
      IADCD=IADCD+1
      NLIST(IADCD)=NFUNC
      NADR(NFUNC)=IADCD
      IADCD=IADCD+1
      NLIST(IADCD)=2
      IADCD=IADCD+1
      NLIST(IADCD)=0
      IADCD=IADCD+1
      NLIST(IADCD)=1
      IADCD=IADCD+1
      NLIST(IADCD)=1
      IADCD=IADCD+1
      NLIST(IADCD)=1
      IADCD=IADCD+1
      NLIST(IADCD)=ID1
      IADCD=IADCD+1
      NLIST(IADCD)=-18
      IADCD=IADCD+1
      NLIST(IADCD)=-15
      IADCD=IADCD+1
      IF(.NOT. LTHETA) GO TO 48
      NPRIOR(MAXF-1)=NFUNC
      NPRS(NFUNC-1)=MAXF
      NPRIOR(MAXF)=NFUNC-1
      NPRS(NFUNC)=MAXF-1
      IF(LTHETA .OR. JACOB) GO TO 16
   48 ITAN=1
      NTAN=NTAN+1
      GO TO 16
   15 IADCD=IADCD+1
      NLIST(IADCD)=ID1
      IADCD=IADCD+1
C             FUNCTION CORRESPONDS TO PARTIAL D(FJ)/D(XI)
   16 IF(ID1 .LE. 1000) GO TO 17
      IC=ID1-1000
      ICC=NDER(IC,IVAR)
      IF(ICC .GT. 1000) GO TO 41
      IDNT=IDNT-1
      GO TO 35
   41 NLIST(IADCD)=ICC
      IADCD=IADCD+1
C             INSERT EXTRA TERM FOR THE EXPONENT
   17 IF(ID2 .GE. 0) GO TO 25
   42 IF(ID .GT. 5) GO TO 18
      NLIST(IADCD)=ID
      IADCD=IADCD+1
C             REPEATS SPECIFICATION OF FK
   18 NLIST(IADCD)=ID1
      IDNT=IDNT+1
      IADCD=IADCD+1
      IF(ID2 .GE. -26) GO TO 19
      MAXCON=MAXCON+1
      IC=-ID2-26
C             (PJ-1) IS HELD AS A NEW CONSTANT
      CONS(MAXCON)=CONS(IC)-1.0
      CONST=CONS(IC)
      NLIST(IADCD)=-26-MAXCON
      IADCD=IADCD+1
      GO TO 20
C             IF X**2 NO EXPONENT IN DERIVATIVE
   19 NLIST(IADCD)=ID2+1
      IADCD=IADCD+1
      IF(ID2 .EQ. -18) IADCD=IADCD-1
      IC=-ID2-16
      CONST=FLOAT(IC)
   20 MAXCON=MAXCON+1
      IF(ICLIST .GT. 1) GO TO 24
      IF(ICLIST .LT. -1) GO TO 22
      IF(ICLIST .EQ. -1) CONST=-CONST
      GO TO 23
   22 ICLIST=-ICLIST
      CONST=CONST*(-CONS(ICLIST-1))
      GO TO 23
   24 CONST=CONST*CONS(ICLIST-1)
C           NEW CONSTANT CI*PJ
   23 CONS(MAXCON)=CONST
      NLIST(IFACC+1)=MAXCON+1
C
C           SIMPLIFY IF CONSTANT ONLY FOR DERIVATIVE FACTOR
C
   25 IF(J .EQ. NFACT) GO TO 31
      IF(ID1 .LE. 1000) GO TO 39
      IF(ICC .GT. 1000) GO TO 39
   35 IF(ICC .GT. 1) GO TO 33
      IF(ICC .LT. -1) GO TO 32
      IF(ICC .EQ. 1) CONST=1.0
      IF(ICC .EQ. -1) CONST=-1.0
      GO TO 34
   33 CONST=CONS(ICC-1)
      GO TO 34
   32 ICC=-ICC
      CONST=-CONS(ICC-1)
   34 MAXCON=MAXCON+1
      IF(ICLIST .GT. 1) GO TO 37
      IF(ICLIST .LT. -1) GO TO 36
      IF(ICLIST .EQ. -1) CONST=-CONST
      GO TO 38
   36 ICLIST=-ICLIST
      CONST=CONST*(-CONS(ICLIST-1))
      GO TO 38
   37 CONST=CONST*CONS(ICLIST-1)
   38 CONS(MAXCON)=CONST
      NLIST(IFACC+1)=MAXCON+1
      ICLIST=MAXCON+1
      IF(ID2 .LT. 0) GO TO 42
   39 IF(J .EQ. NFACT) GO TO 31
      ISWIT=1
      ICC=IADC+1
      IMAX=ICC+1
      ICOP=IMAX
      IC=1
      LJUMP=.FALSE.
      IF(J .GT. 1) GO TO 47
      ID=NLIST(ICC)
      GO TO 27
   47 IFACT=J
      IFLAG=0
      GO TO 7
   27 IF(ID .GT. 5) GO TO 26
      ICC=ICC+1
      NLIST(IADCD)=ID
      IADCD=IADCD+1
      ID=NLIST(ICC)
   26 IC=IC+1
```

```
      NLIST(IADCD)=ID
      ICC=ICC+1
      IADCD=IADCD+1
   29 ID=NLIST(ICC)
      IF(ID .GE. 0) GO TO 30
      ICC=ICC+1
      IF(ID .NE. -16) GO TO 28
      LJUMP=.TRUE.
      ICC=NLIST(ICC)
      GO TO 29
   28 IPWR=ICC-1
      IF(JC(I) .EQ. 0) GO TO 87
      KK=JC(I)
      IF((KK .EQ. 1) .AND. (JUMPAD(I,KK) .EQ. 0)) GO TO 87
      DO 94 JK=1,KK
      KC=JUMPAD(I,JK)
      IF(KC .EQ. 0) GO TO 94
      KC=NLIST(KC+1)
      IF(KC .EQ. IPWR) GO TO 89
   94 CONTINUE
      GO TO 87
   89 IF(LJUMP) GO TO 87
      GO TO 30
   87 NLIST(IADCD)=ID
      IADCD=IADCD+1
      ID=NLIST(ICC)
   30 IF(IC .LT. NFACT) GO TO 27
      IMAX=ICC
   31 IF(SKIP) GO TO 97
      NTERMD=NTERMD+1
      NFACTD=NFACT+IDNT
      NLIST(IFACC)=NFACTD
   97 CONTINUE
      IADC=IADC+1
  100 CONTINUE
C
C            CHECK IF DERIVATIVE IS CONSTANT OR ZERO .
C
      IF(NTERMD .EQ. 0) GO TO 102
      IF((NTERMD .EQ. 1) .AND. (NFACTD .EQ. 0)) GO TO 103
      GO TO 101
  102 NFUNC=NFUNC-1
      MAXF=MAXF-1
      IF(JACOB) GO TO 107
  106 NDER(IFUNC,IVAR)=0
  108 IADCD=IADCD-2
      IF(ICOUNT .GT. 1) RETURN
      WRITE(6,401) IFUNC,IVAR
  401 FORMAT(1HO,'DF',I2,'/DX',I1,' = 0')
      GO TO 105
  107 IF(.NOT. IREC) IFUNC=I
      IF(NQ .GT. 10 .OR. KPARAM .GT. 50) GO TO 125
      NDJ(I,IVAR,KVAR)=0
      IF(.NOT. IREC .AND. NFLAG .EQ. 1 .AND. I .LE. NINTF)
     +NDER(KFUNC,IVAR)=0
      IF(I .LE. NINTF) NDER(KFUNC,IVAR)=0
```

```
    IVAR=KVAR
    GO TO 126
125 IVAR=KVAR
    NDERJ(IFUNC,IVAR)=0
126 IF(IREC) NDER(KFUNC,K)=0
    GO TO 108
103 NFUNC=NFUNC-1
    MAXF=MAXF-1
    IF(JACOB) GO TO 120
121 ICLIST=NLIST(IADCD-1)
    IF(JACOB) GO TO 122
    NDER(IFUNC,IVAR)=ICLIST
    GO TO 123
122 IF(NQ .GT. 10 .OR. KPARAM .GT. 50) NDERJ(IFUNC,IVAR)=ICLIST
    IF(I .LE. NINTF) NDER(KFUNC,K)=ICLIST
    IF(IREC) NDER(KFUNC,K)=ICLIST
123 IADCD=IADCD-4
    IF(ICLIST .EQ. 1) GO TO 110
    IF(ICLIST .EQ. -1) GO TO 109
    IF(ICLIST .GT. 1) GO TO 111
    IF(ICLIST .LT. -1) GO TO 112
109 CONST=-1.0
    GO TO 115
110 CONST=1.0
    GO TO 115
111 CONST=CONS(ICLIST-1)
    GO TO 115
112 ICLIST=-ICLIST
    CONST=-CONS(ICLIST-1)
115 IF(ICOUNT .GT. 1) RETURN
    WRITE(6,402) IFUNC,IVAR,CONST
402 FORMAT(1HO,'DF',I2,'/DX',I1,' = ',F8.4)
    GO TO 105
120 IF(.NOT. IREC) IFUNC=I
    IF(NQ .GT. 10 .OR. KPARAM .GT. 50) GO TO 127
    NDJ(I,IVAR,KVAR)=NLIST(IADCD-1)
    IF(.NOT. IREC .AND. NFLAG .EQ. 1 .AND. I .LE. NINTF)
   +NDER(KFUNC,IVAR)=NLIST(IADCD-1)
127 IVAR=KVAR
    GO TO 121
101 NLIST(MAXAD+2)=NTERMD
    MAXAD=IADCD-1
    IF(ICOUNT .GT. 1) RETURN
    WRITE(6,400) IFUNC,IVAR,(NLIST(J),J=L,MAXAD)
400 FORMAT(1HO,'DF',I2,'/DX',I1,2X,20I4)
    WRITE(6,550) MAXF,NFUNC,NFUNC,MAXF
550 FORMAT(1HO,'NPRIOR(',I2,') = ',I2,5X,'NPRS(',I2,') = ',I2)
105 RETURN
    END
```

```
      SUBROUTINE EVAL(IADC,I,IFUNC,VFUNC,IT,MAXAD,NPARAM,V,VFLIST)
      COMMON X(100,50)
      COMMON /A1/NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),NADR(300
     I),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      REAL NDERS,NDERJS
      DIMENSION V(NPARAM)
      DIMENSION VFLIST(200)
      LOGICAL LJUMP
      LJUMP=.FALSE.
      NTERM=NLIST(IADC)
      IF(NTERM .EQ.O) RETURN
      IADC=IADC+1
      DO 100 I1=1,NTERM
      VTERM=1.
      NFACT=NLIST(IADC)
      IADC=IADC+1
      ICLIST=NLIST(IADC)
      IF(NFACT .EQ. 0) GO TO 96
      GO TO 95
   96 IADC=IADC+1
      IF(ICLIST .GE. 0) GO TO 80
      IF(ICLIST .EQ. -1) GO TO 82
      ICLIST=-ICLIST
      VFUNC=VFUNC-CONS(ICLIST-1)
      GO TO 100
   82 VFUNC=-1.+VFUNC
      GO TO 100
   80 IF(ICLIST .GT. 1) GO TO 81
      VFUNC=1.+VFUNC
      GO TO 100
   81 VFUNC=VFUNC+CONS(ICLIST-1)
      GO TO 100
   95 DO 97 J=1,NFACT
      IADC=IADC+1
      ID=NLIST(IADC)
      IF(ID .GT. 5) GO TO 1
      IADC=IADC+1
      ID1=NLIST(IADC)
      GO TO 2
    1 ID1=ID
    2 IF(IADC .EQ. MAXAD) GO TO 84
      ID2=NLIST(IADC+1)
      IF(ID2 .GE. 0) GO TO 3
      IADC=IADC+1
      IF(ID2 .EQ. -16) GO TO 8
      IPWR=IADC
      IF(JC(I) .EQ. 0) GO TO 3
      KK=JC(I)
      IF((KK .EQ. 1) .AND. (JUMPAD(I,KK) .EQ. 0)) GO TO 3
      DO 93 JK=1,KK
      KC=JUMPAD(I,JK)
      IF(KC .EQ. 0) GO TO 93
      KC=NLIST(KC+1)
      IF(KC .EQ. IPWR) GO TO 91
   93 CONTINUE
```

```
      GO TO 3
   91 IF(LJUMP) GO TO 3
   84 ID2=0
    3 IF(ID1 .GT. 1000) GO TO 4
      IC=ID1-5
      IF(IC .LE. NPARAM) GO TO 86
      VFACT=X(IT,IC-NPARAM)
      GO TO 94
   86 VFACT=V(IC)
      GO TO 94
    4 NFUNC=ID1-1000
      VFACT=VFLIST(NFUNC)
      GO TO 94
    8 LJUMP=.TRUE.
      IADC=NLIST(IADC+1)-1
      GO TO 2
    9 IF(ID .GT. 5) GO TO 99
      GO TO(10,11,12,13,14),ID
   10 VFACT=ALOG(VFACT)
      GO TO 99
   11 VFACT=EXP(VFACT)
      GO TO 99
   12 VFACT=SIN(VFACT)
      GO TO 99
   13 VFACT=COS(VFACT)
      GO TO 99
   14 VFACT=ATAN(VFACT)
      GO TO 99
   94 IF(ID2 .GE. 0) GO TO 9
      IF(ID2 .EQ. -15) GO TO 98
      IF(ID2 .GE. -26) GO TO 19
      ICONST=-ID2-26
      CONST=CONS(ICONST)
      VFACT=VFACT**ICONST
      GO TO 9
   19 IC=-ID2-16
      CONST=FLOAT(IC)
      IF(IC .GT. 0) GO TO 200
      IC=-IC
      VFACT=1./VFACT**IC
      GO TO 9
  200 VFACT=VFACT**IC
      GO TO 9
C           TEST DIVISION SYMBOL BELONGS TO CURRENT FUNCTION
   98 VFACT=1./VFACT
      GO TO 9
   99 VTERM=VTERM*VFACT
   97 CONTINUE
      IF(ICLIST .GE. 0) GO TO 21
      IF(ICLIST .EQ. -1) GO TO 21
      ICLIST=-ICLIST
      CONST=-CONS(ICLIST-1)
      GO TO 22
   21 CONST=FLOAT(ICLIST)
      IF((ICLIST .EQ. 1) .OR. (ICLIST .EQ. -1)) GO TO 22
      CONST=CONS(ICLIST-1)
   22 VFUNC=VFUNC+VTERM*CONST
      IADC=IADC+1
  100 CONTINUE
      RETURN
      END
      SUBROUTINE INPUT(N,NL,NVAR,NR,NTRAN)
      DIMENSION XL(6,60)
      DIMENSION NAME(100)
      COMMON X(100,50)
      NVAR=NL*NR
      NA=N+NL-1
      DO 45 I=1,NA
      READ(5,50) (X(I,J),J=1,NR)
   50 FORMAT(8F10.4)
   45 CONTINUE
      IF(NTRAN .EQ. 0) GO TO 10
      CALL DATALT(N,NR,NVAR,NAME)
   10 IF(NL-1 .LE. 0) GO TO 14
      DO 6 I=1,NL
      DO 6 J=1,NVAR
    6 XL(I,J)=X(I,J)
      MK=0
      DO 7 I=1,N
      DO 7 J=1,NR
      IJ=I+NL-1
    7 X(I,J)=X(IJ,J)
      DO 13 K=2,NL
      MK=MK+NR
      NC=N-K+1
      DO 11 I=1,NC
      DO 11 J=1,NR
      IK=I+K-1
      IJ=J+MK
      K1=K-1
      DO 12 IN=1,K1
      IT=NL-K+IN
   12 X(IN,IJ)=XL(IT,J)
   11 X(IK,IJ)=X(I,J)
   13 CONTINUE
   14 WRITE(6,15)
   15 FORMAT(1H1,10X,'DATA'///)
      DO 52 I=1,N
      WRITE(6,27) (X(I,J),J=1,NVAR)
   27 FORMAT(1H ,10F10.4)
   52 CONTINUE
      RETURN
      END
      SUBROUTINE DATALT(N,NR,NVAR,NAME)
      DIMENSION NAME(100)
      COMMON X(100,50)
      READ(5,888) KD,IDA
  888 FORMAT(20I4)
      READ(5,10) (NAME(I),I=1,KD)
   10 FORMAT(20A4)
      DO 15 J=1,IDA
      READ(5,11) NOP,NA,NB,NC,VAL
   11 FORMAT(4I4,F8.4)
      IF(NOP .NE. 10) GO TO 40
      IVAL=IFIX(VAL)
      ND=NC-1
      CALL ALMLAG(ND,N,NB,IVAL,NA)
      GO TO 15
   40 IF(NB .NE. 0) WRITE(6,7) NOP,NA,NAME(NA),NB,NAME(NB),NC,NAME(NC)
      IF(NB .EQ. 0) WRITE(6,18) NOP,NA,NAME(NA),NC,NAME(NC)
      IF(NOP .EQ. 6 .OR. NOP .EQ. 7) X(1,NC)=VAL
      IF(NOP .EQ. 3 .AND. VAL .EQ. 0.) VAL=1.
      IF(NOP .EQ. 4 .AND. VAL .EQ. 0.) VAL=1.
      DO 30I=1,N
      SP=0.
      SQ=1.
      GO TO (1,2,3,4,5,6,6,8,9),NOP
    1 IF(NB .NE. 0) SP=X(I,NB)
      X(I,NC)=X(I,NA)+SP+VAL
      GO TO 30
    2 X(I,NC)=X(I,NA)-X(I,NB)+VAL
      GO TO 30
    3 IF(NB .NE. 0) SQ=X(I,NB)
      X(I,NC)=X(I,NA)*SQ*VAL
      GO TO 30
    4 IF(X(I,NB) .EQ. 0) WRITE(6,25) NOP,NB
      IF(X(I,NB) .EQ. 0.) GO TO 15
      X(I,NC)=X(I,NA)*VAL/X(I,NB)
      GO TO 30
    5 IF(X(I,NA) .LE. 0.) WRITE(6,25) NOP,NA
      IF(X(I,NA) .GT. 0) X(I,NC)=ALOG(X(I,NA))
      GO TO 30
    6 X(I+1,NC)=X(I,NA)
      WRITE(6,25) NOP,NA
      IF(NOP .NE. 7) GO TO 30
      X(I,NB)=X(I,NA)-X(I,NC)
      GO TO 30
    8 X(I,NC)=EXP(X(I,NA))
      GO TO 30
    9 IF(X(I,NA) .LE. 0.) WRITE(6,25) NOP,NA
      IF(X(I,NA) .GT. 0.) X(I,NC)=SQRT(X(I,NA))
   30 CONTINUE
   15 CONTINUE
   25 FORMAT(1HO,' ILLEGAL OPERATION FOR ',I4,2X,' ON VARIABLE ',I4)
    7 FORMAT(1HO,' OPERATION',I4,' PERFORMED ON VARIABLES',I4,'  (',
     IA4,'  ) AND ',I4,'  (',A4,' ) TO CREATE VARIABLE',I4,'  (',A4,
     I'  )')
   18 FORMAT(1HO,' OPERATION',I4,'  PERFORMED ON VARIABLE',I4,'  (',A4,
     I'  ) TO CREATE VARIABLE',I4,'  (',A4,'  )')
      NVAR=KD
      RETURN
      END
  SUBROUTINE ALMLAG(ND,N,NB,IVAL,NA)
  COMMON X(100,50)
  ITNEW=N-NB
  LOPP=IVAL+1
  ML1=NB+1
  DO 1 I=1,ITNEW
  IMAXL=I+NB
  DO 2 J=1,LOPP
  NJ=ND+J
  JO=J-1
  S=0.
  DO 3 K=1,ML1
  KO=K-1
3 S=S+X(IMAXL-KO,NA)*(ML1-KO)**JO
2 X(IMAXL,NJ)=S
1 CONTINUE
  N=N+LOPP
  RETURN
  END
```

```
      SUBROUTINE FUNML(NPARAM,V,FV)
      COMMON X(100,50)
      COMMON /A1/ NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),
     1NADR(300),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     1ICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     1IADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      DIMENSION V(NPARAM)
      LOGICAL LTHETA,JACOB
      IF(ICOUNT .GT. 1 .AND.(NQ .LE. 10 .OR. KPARAM .LE. 50)) GO TO 151
      IF(IMETH .EQ. 0 .AND. (NQ .LE. 10 .OR. KPARAM .LE. 50)) GO TO 151
      IF(IMETH .EQ. 0) GO TO 152
      LTHETA=.FALSE.
      JACOB=.FALSE.
      CALL DIFIML(NPARAM,V)
  152 DO 155 K1=1,NPARAM
      K=K1
      LTHETA=.TRUE.
      CALL DIFIML(NPARAM,V)
      JACOB=.TRUE.
      CALL DIFIML(NPARAM,V)
      JACOB=.FALSE.
  155 CONTINUE
  151 DO 150 K1=1,NPARAM
      K=K1
      CALL DIEVAL(NPARAM,V)
      CALL PQEVAL(NPARAM,V)
  150 CONTINUE
      FV=-(DETJT-0.5*FLOAT(NT)*ALOG(DETF))
      MFUN=MFUN+1
      RETURN
      END
      SUBROUTINE GCHECK(NPARAM,V,FUN,FUNCT)
      COMMON X(100,50)
      COMMON /A1/ NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),
     INADR(300),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      DIMENSION V(NPARAM)
      DIMENSION STORE(50)
      EXTERNAL FUNCT
      DATA EPS/1.E-3/
      DO 10 I=1,NPARAM
      V(I)=V(I)+EPS
      CALL FUNCT(NPARAM,V,FV)
      FHI=FV-FUN
      FPLUS=FV
      V(I)=V(I)-EPS*2.
      CALL FUNCT(NPARAM,V,FV)
      FLO=FUN-FV
      FMUS=FV
      V(I)=V(I)+EPS
      STORE(I)=(FPLUS-FMUS)/(2.*EPS)
   10 CONTINUE
      WRITE(6,9002) (STORE(I),I=1,NPARAM)
 9002 FORMAT(1HO,'APPROXIMATE GRADIENT ',10F10.4)
      RETURN
      END
      SUBROUTINE GSTEP(FUN,FV,GRAD,SC,NPARAM,V,FUNCT,IFOK)
      COMMON X(100,50)
      COMMON /A1/ NLIST(4000),NPRIOR(300),NPRS(300),NDER(300,60),
     INADR(300),LISTEN(20),JUMPAD(20,5),JC(20),CONS(200)
      COMMON /A2/ VMU(100,50),R(50,50),D(50),TEMP(50)
      COMMON /A3/ LTMAX,LMAXF,JTMAXF,LTFUNC(50),JMAXF,JFUNC(50),
     IICOUNT,DETF,DETJT
      COMMON /A4/ NQ,NB,NI,MFUN,NT,K,KVAR,KFUNC,KPARAM,IMETH,ISTEP,NINTF
      COMMON /A5/ LTHETA,JACOB,IREC,MAXAD,MAXF,MAXCON,IVECT(70),IADC,
     IIADCD,IFUNC,NFUNC,ITAN,NTAN,NFLAG,LDIFF,ICON(4)
      COMMON /A6/ VLF(300,100),NDERS(20,50),NDERJ(300,60),NDERJS(20,20)
      COMMON /A7/ NDJ(10,50,10)
      REAL NDERS,NDERJS
      EXTERNAL FUNCT
      DIMENSION V(NPARAM)
      LOGICAL LTHETA,JACOB,IFOK
      IFOK=.TRUE.
      IDC=0
      IQ=1
      PREC=.5E-11
      E1=.01
      E2=.7
      SL=0.
      DL=1.
      FL=FUN
      DF=PREC*(ABS(FL)+PREC)
      IKT=0
      FV=FUN
      DO 1 I=1,NPARAM
    1 V(I)=TEMP(I)-SC*D(I)
      CALL FUNCT(NPARAM,V,FV)
      IF(FV .GT. FUN) GO TO 94
C
C          EXTRAPOLATE TO BRACKET MINIMUM
C
   93 IKT=IKT+1
      FO=-SC*GRAD
      DD=(FV-(FUN+FO))/FO+1.0
      IF(DD .LE. E2) GO TO 3
      IF(FV .GE. FL) GO TO 3
      IF(IKT .GT. 1 .AND. ABS(1.0-DD) .GE. E1) GO TO 3
      SL=SC
      DL=DD
      FL=FV
      IF(IKT .GT. 5) GO TO 13
      IF(DD .GE. .95) SC=10.0*SC
      IF(DD .LT. .95) SC=.5*SC/(1.0-DD)
      DO 2 I=1,NPARAM
    2 V(I)=TEMP(I)-SC*D(I)
      CALL FUNCT(NPARAM,V,FV)
      GO TO 93
    3 IF(DD .GE. E1) GO TO 14
      IF(ABS(1.0-DL) .GE. E1) GO TO 13
      GO TO 4
C
C          MINIMUM BRACKETED
```

```
C
   94 FO=-SC*GRAD
      DD=(FV-(FUN+FO))/FO+1.0
      IF(DD .LT. E1) GO TO 4
      IF(ABS(1.0-DD) .GE. E1) GO TO 14
      SL=SC
      DL=DD
      FL=FV
      IF(IQ .EQ. 0) GO TO 7
      GO TO 5
    4 SR=SC
      DR=DD
      FR=FV
      IF(ABS(SC*GRAD) .LE. DF) GO TO 7
C
C          CHECK SIZE OF BRACKET
C
    5 IF((SR-SL) .LE. PREC*SR) GO TO 13
      SC=SL+(SR-SL)*AMAX1(.001,(.5-DL)/(DR-DL))
      IQ=0
      DO 6 I=1,NPARAM
    6 V(I)=TEMP(I)-SC*D(I)
      CALL FUNCT(NPARAM,V,FV)
      GO TO 94
C
C          USE MIDPOINT OF INTERVAL IF QUADRATIC INTERPOLATION FAILS
C
    7 SC=.5*(SR+SL)
      DO 8 I=1,NPARAM
    8 V(I)=TEMP(I)-SC*D(I)
      CALL FUNCT(NPARAM,V,FV)
      IF(FV .LT. FUN) GO TO 9
      IF(ABS(SR*GRAD) .GT. DF) GO TO 9
C
C          RECALCULATE PROJECTED GRADIENT
C
      IF(SL .GT. 0) GO TO 13
      IF(IDC .EQ. 1) GO TO 13
      IDC=1
      GDL=GRAD
      GRAD=-(4.0*FV-FR-3.0*FUN)/SR
      IF(GRAD .LE. 0) GO TO 10
      DR=DR*GDL/GRAD
    9 IQ=1
      GO TO 94
C
C          EXPLORE REVERSE SEARCH DIRECTION
C
   10 IF(GRAD .EQ. 0) GO TO 13
      DO 11 I=1,NPARAM
   11 V(I)=TEMP(I)+SC*D(I)
      CALL FUNCT(NPARAM,V,FT)
      IF(FT .GE. FUN) GO TO 13
      DO 12 I=1,NPARAM
   12 D(I)=-D(I)
      GRAD=(FV-FT)/SC
      DL=1.0
      SL=0.0
      FV=FT
      FL=FUN
      IKT=0
      GO TO 93
C
C            EXIT WHEN TERMINATION CONDITION NOT MET AT SC
C
   13 SC=SL
      FV=FL
   14 DO 15 I=1,NPARAM
   15 V(I)=TEMP(I)-SC*D(I)
      IF(FV .GE. FUN) IFOK=.FALSE.
      RETURN
      END
```

APPENDIX C

A User's Guide to NLMLE

To illustrate how to use NLMLE with the specifications defined in Chapter 5, consider the following model:

$$y_{1t} = (\theta_1\theta_3 - \tfrac{1}{2}\theta_2)y_{2t} + \frac{\theta_1}{\theta_2} y_{1,t-1} + 2\theta_3^2 z_{1t}$$

$$+ \theta_3\theta_4 z_{2t} + u_{1t}$$

$$y_{2t} = \theta_4 y_{1t} + \theta_5 z_{3t} + u_{2t}$$

Assume we have 60 observations in the data and the starting values of the coefficients are also given.

Rewrite model as:

$$u_{1t} = y_{1t} - (\theta_1\theta_3 - \tfrac{1}{2}\theta_2)y_{2t} - \frac{\theta_1}{\theta_2} y_{1,t-1} - 2\theta_3^2 z_{1t} - \theta_3\theta_4 z_{2t}$$

$$u_{2t} = y_{2t} - \theta_4 y_{1t} - \theta_5 z_{3t}$$

Now transform all the equations and variables into NLMLE specifications:

1. Equations: $\{u_1, u_2\} \rightarrow \{F_1, F_2\}$
2. Parameters set: $\{\theta_1, \theta_2, \theta_3, \theta_4, \theta_5\} \rightarrow \{v_1, v_2, v_3, v_4, v_5\}$
3. Endogenous variables: $\{y_{1t}, y_{2t}\} \rightarrow \{v_6, v_7\}$
4. Predetermined variables: $\{z_{1t}, z_{2t}, z_{3t}, y_{1,t-1}\} \rightarrow \{v_8, v_9, v_{10}, v_{11}\}$.

The transformed model now becomes:

$$F1 = v_6 - (v_1 * v_3 - \tfrac{1}{2} * v_2) * v_7 - (v_1/v_2) * v_{11}$$

$$- 2 * v_3 * v_3 * v_8 - v_3 * v_4 * v_9$$

$$F2 = v_7 - v_4 * v_6 - v_5 * v_{10}.$$

Notice that powers can be expressed as "**", e.g. θ_3^2 as v_3 ** 2.

Input Instructions

(1)	BHHH	GSTEP	(2I4)							
	0	0								
(2)	IMAX	TOLB	(I4,F10.4)							
	50	0.0001								
(3)	NB	NI	NINTF	NY	NZ	N	NT	NL	NVAR	(20I4)
	2	0	0	2	4	5	60	1	6	

(4) Names of Variables (20A4)

y_{1t} y_{2t} z_{1t} z_{2t} z_{3t} $y_{1t\ell}$.

(5) Data series, input ordering as (4) by variables (8F10.4) i.e. the X matrix.

(6) Starting values of parameters (8F10.4) i.e. $\{\theta_1,\ldots,\theta_5\}$ i.e. the V vector.

(7) Equations: $\left.\begin{array}{l}\text{F1} = \\ \text{F2} = \end{array}\right\}$ as above.

(8) \$\$\$\$.

APPENDIX D

Program Output - A Typical Run From Model (iii)

```
NONLINEAR ARCTANGENT MODEL:

METHOD  =  BHHH

STEP  =   GSTEP (MODIFIED LINE SEARCH)

MAXIMUM NUMBER OF ITERATIONS  =  50

TOLERANCE LEVEL FOR CONVERGENCE  =  0.001

5 EQUATIONS   50 OBSERVATIONS   6 PARAMETERS

COEFFICIENTS

      .3   1.0   1.0   5.0   5.0   5.0

INPUT FUNCTIONS:

F1  =  V1 * ATAN (V2 * V7) + V3 * V7 + .1 + V3 ** 2 * V8

F2  =  V1 * ATAN (V2 * V9) + .1 * V3 ** 2 * V7 + V3 * V8

F3  =  V1 * ATAN (V2 * V9) - .1 * V3 ** 2 * V8 + (V3 + .1 * V3 ** 2)
                                                                 * V9

F4  =  V1 * ATAN (V2 * V10) + .1 * V3 ** 2 * V9 + (V3 - .1 * V3 ** 2) * V10

F5  =  V1 * ATAN (V2 * V11) + .1 * V3 ** 2 * V8 + .1 * V3 ** 2 * V10
                                                            + V3 * V11

F6  =  (V4 * V12 + V17 ** 2) + F1

F7  =  (V5 * V13 + V17 ** 2) + F2

F8  =  (V4 * V14 + V18 ** 2) + F3

F9  =  (V6 * V15 + V18 ** 2) + F4

F10 =  (V4 * V16 + V18 ** 2) + V5
```

```
PARAMETERS:  V1  V2  V3  V4  V5  V6

ENDOGENOUS VARIABLES:  V7  V8  V9  V10  V11

EXOGENOUS VARIABLES:   V12  V13  V14  V15  V16  V17  V18

START TIME  =  8.1430


ITERATION NUMBER 1

GRADIENT

-.379390E+03 .212810E+02 -.200745E+04 -.293029E+04 .657361E+03 -.749687E+03

GRADIENT NORM  =  3708.817889

FUN = -940.897488   FUNNEW = -943.141288

STEPSIZE = .100000E + 01   GRAD = .493929E + 01

NCALL = 2

DIRECTION

-.47345E-02 .44575E-01 .52228E-03 -.92267E-03 .11082E-02 .25493E-03

PARAMETER ESTIMATES

.30473E+00 .95543E+00 .99948E+00 .50009E+01 .49989E+01 .49997E+01


ITERATION NUMBER 2

GRADIENT

-.760862E+02 .150458E+00 -.746201E+03 .881762E+03 .241066E+03 -.484311E+03

GRADIENT NORM = 1277.802584

FUN = -943.141288   FUNNEW = -943.445479

STEPSIZE = .441979E+00   GRAD = .136577E+01

NCALL = 4
```

```
DIRECTION

.98958E-02 -.35333E-01 -.21791E-02 .22932E-03 -.82251E-03 -.10201E-02


PARAMETER ESTIMATES

.30036E+00 .97104E+00 .10004E+01 .50008E+01 .49993E+01 .50002E+01



ITERATION NUMBER 3


GRADIENT

-.260989E+02 .776491E+00 -.157761E+03 -.225522E+02 -.102499E+03 -.354972E+02


GRADIENT NORM = 194.537814


FUN = -943.445479   FUNNEW = -943.459954


STEPSIZE = .100000E+01   GRAD = .275175E-01


NCALL = 5


DIRECTION

-.16085E-03 .96259E-03 .77717E-04 -.25802E-04 .33775E-03 .10365E-04


PARAMETER ESTIMATES

.30052E+00 .97008E+00 .10004E+01 .50008E+01 .49989E+01 .50002E+01



ITERATION NUMBER 4


GRADIENT

-.588064E+01 -.899695E+00 -.363169E+02 .268113E+01 .128140E+02 -.563097E+01


GRADIENT NORM = 39.463905


FUN = -943.459954   FUNNEW = -943.460528


STEPSIZE = .453732E+00   GRAD = .253337E+02
```

```
NCALL = 7

DIRECTION

.44748E-03 -.18953E-02 -.93841E-04 .52135E-05 -.14690E-04 -.40123E-04

PARAMETER ESTIMATES

.30032E+00 .97094E+00 .10004E+01 .50008E+01 .49989E+01 .50002E+01


ITERATION NUMBER 5

GRADIENT

-.146527E+01 -.348852E+00 -.654604E+01 -.175159E+02 .587007E+01 .110445E+02

GRADIENT NORM = 22.546955

FUN = -943.460428   FUNNEW = -943.460633

STEPSIZE = .100000E+01   GRAD = .346181E-03

NCALL = 8

DIRECTION

-.48335E-04 .80070E-04 .15275E-04 -.46903E-05 .32733E-04 .11678E-04

PARAMETER ESTIMATES

.30037E+00 .97086E+00 .10004E+01 .50008E+01 .49989E+01 .50002E+01


ITERATION NUMBER 6

GRADIENT

-.146241E+01 -.891401E-01 -.984296E+01 .129665E+02 .300475E+01 -.757161E+01

GRADIENT NORM = 18.262456
```

```
FUN = -943.460633   FUNNEW = -943.460688

STEPSIZE = .375083E+00   GRAD = .297599E-03

NCALL = 10

DIRECTION

.14706E-03 -.58491E-03 -.31749E-04 .43311E-05 -.12071E-04 -.16921E-04

PARAMETER ESTIMATES

.30031E+00 .97108E+00 .10004E+01 .50008E+01 .49989E+01 .50002E+01


ITERATION 7

GRADIENT

-.269233E+00 -.181003E+01 -.127856E+01 .465367E+00 .107269E+01 .395240E-01

GRADIENT NORM = 1.753947

FUN =  -943.460688   FUNNEW = -943.460688

STEPSIZE = .375083+00   GRAD = .297599E-03

NCALL = 10

DIRECTION

-.29042E-05 -.53806E-06 .14347E-05 -.62081E-08 .43648E-05 .42346E-06

PARAMETER ESTIMTES

.30031E+00 .97108E+00 .10004E+01 .50008E+01 .49989E+01 .50002E+01


CONVERGENCE ACHIEVED AFTER 7 ITERATIONS.

NUMBER OF FUNCTION EVALUATIONS = 10

LOG LIKELIHOOD FUNCTION = -943.460688
```

```
INVERSE HESSIAN MATRIX

 .000099
-.000363   .001705
-.000021   .000072   .000005
 .000001  -.000007  -.000000   .000000
-.000009   .000025   .000003  -.000000   .000006
-.000009   .000032   .000002  -.000000   .000001   .000001


PARAMETERS              STD -ERRORS              T-RATIOS

  .300312                 .009934               30.230912
  .971079                 .041293               23.516612
 1.000402                 .002251              444.500513
 5.000848                 .000504             9921.666183
 4.998896                 .002478             2017.202929
 5.000198                 .001148             4346.444014


END TIME  =  21.0350
```

APPENDIX E

A Parallel Inversion Routine

```
      REAL JT(,,N,N), UNIT_MATRIX (,,N,N), DET_JT(,), PIVOT_ELEMENT (,),
     +COLUMN_PIVOT (,,N), SIGMA (,), TEMP (,), AA(,), ATEMP (,),
     +BETEMP (,)
      LOGICAL SWAP (,), SIGN_CHANGE (,)
      EQUIVALENCE (AA, TEMP), (PIVOT_ELEMENT, ATEMP, BETEMP)
C
C           INITIALISE UNIT MATRIX
C
      DET_JT = 1.0
      DO 10 I = 1, N
      DO 10 J = 1, N
      UNIT_MATRIX (,,I,J) = 0.0
      IF(I.EQ.J) UNIT_MATRIX (,,I,I) = 1.0
   10 CONTINUE
C
C           SELECT PIVOT COLUMN AND PIVOT ELEMENT
C
      DO 90 K = 1, N-1
      COLUMN_PIVOT (,,K) = K
      PIVOT_ELEMENT = JT(,,K,K)
      K1 = K + 1
      DO 30 I = K1, N
      SWAP = ABS(PIVOT_ELEMENT) - ABS(JT(,,I,K)).LT.0.0
      PIVOT_ELEMENT (SWAP) = JT(,,I,K)
   30 COLUMN_PIVOT (SWAP,K) = I
```

```
C
C           CHECK FOR SINGULARITY
C
      IF (ALL(PIVOT_ELEMENT.NE.0.0)) GO TO 40
      DET_JT(PIVOT_ELEMENT.EQ.0.0) = 0.0
      RETURN
C
C           INTERCHANGE COLUMNS
C
   40 DO 50 I = K1, N
      SWAP = COLUMN_PIVOT (,,K).EQ.I
      IF (.NOT.ANY(SWAP)) GO TO 50
      DO 45 J = 1, N
      TEMP = JT(,,K,J)
      JT(SWAP,K,J) = JT(,,I,J)
      JT(SWAP, I,J) = TEMP
      TEMP = UNIT_MATRIX (,,K,J)
      UNIT_MATRIX (SWAP,K,J) = UNIT_MATRIX (,,I,J)
   45 UNIT_MATRIX (SWAP,I,J) = TEMP
   50 CONTINUE
C
C           DIVIDE COLUMN BY PIVOT
C
      DO 60 J = 1, N
      JT(,,K,J) = JT(,,K,J)/PIVOT_ELEMENT
   60 UNIT_MATRIX (,,K,J) = UNIT_MATRIX (,,K,J)/PIVOT_ELEMENT
C
C           REDUCE MATRIX
C
```

```
      DO 80 I = K1, N
      AA = JT(,,I,K)
      DO 65 J = K, N
   65 JT(,,I,J) = JT(,,I,J) - AA * JT(,,K,J)
      DO 70 J = 1, N
   70 UNIT_MATRIX (,,I,J) = UNIT_MATRIX (,,I,J) - AA * UNIT_MATRIX (,,K,J)
   80 CONTINUE
C
C           CALCULATE DETERMINENT
C
      SIGN_CHANGE = .FALSE.
      DO 85 I = K1, N
   85 SIGN_CHANGE = SIGN_CHANGE .OR. (COLUMN_PIVOT (,,I).EQ.I)
      PIVOT_ELEMENT (SIGN_CHANGE) = - PIVOT_ELEMENT
   90 DET_JT = DET_JT * PIVOT_ELEMENT
      DET_JT = DET_JT + JT(,,N,N)
C
C           BACK SUBSTITUTION
C
      ATEMP = JT(,,N,N)
      DO 95 J = 1, N
   95 JT(,,N,J) = UNIT_MATRIX (,,N,J)/ATEMP
      DO 120 I = 2, N
      II = N+1 - I
      IIP1 = II + 1
      AA = JT(,,II,II)
      DO 100 J = IIP1, N
  100 UNIT_MATRIX (,,N,J) = JT(,,II,J)
      DO 110 J = 1, N
```

```
     SIGMA = 0.0
     DO 105 K = IIP1, N
105  SIGMA = SIGMA + UNIT_MATRIX (,,N,K) * JT(,,K,J)
110  JT(,,II,J) = (UNIT_MATRIX (,,II,J) - SIGMA)/AA
120  CONTINUE
```

APPENDIX F

Sets of Non-linear Models

(a) Model (ii), $n = 5$, $p = 12$

The model is:

$$f_1^*(y_t) = \gamma_1 \tan^{-1}(\alpha y_{1t}) + \theta_1 y_{1t} + 0.1 * \theta_1^2 y_{2t}$$

$$f_2^*(y_t) = \gamma_2 \tan^{-1}(\alpha y_{2t}) + 0.1 * \theta_1^2 y_{1t} + \theta_1 y_{2t}$$

$$f_3^*(y_t) = \gamma_3 \tan^{-1}(\alpha y_{3t}) - 0.1 * \theta_1^2 y_{2t} + (\theta_1 + 0.1 * \theta_1^2) y_{3t}$$

$$f_4^*(y_t) = \gamma_4 \tan^{-1}(\alpha y_{4t}) + 0.1 * \theta_1^2 y_{3t} + (\theta_1 - 0.1 * \theta_1^2) y_{4t}$$

$$f_5^*(y_t) = \gamma_5 \tan^{-1}(\alpha y_{5t}) + 0.1 * \theta_1^2 y_{2t} + 0.1 * \theta_1^2 y_{4t} + \theta_1 y_{5t}$$

and

$$u_{1t} = (\eta_{11} z_{1t} + z_{6t}^2) + f_1^*(y_t)$$

$$u_{2t} = (\eta_{22} z_{2t} + z_{6t}^2) + f_2^*(y_t)$$

$$u_{3t} = (\eta_{33} z_{3t} + z_{7t}^2) + f_3^*(y_t)$$

$$u_{4t} = (\eta_{44} z_{4t} + z_{7t}^2) + f_4^*(y_t)$$

$$u_{5t} = (\eta_{55} z_{5t} + z_{7t}^2) + f_5^*(y_t)$$

(b) Model (iii), $n = 5$, $p = 6$

The model is:

$$f_1^*(y_t) = \gamma \tan^{-1}(\alpha y_{1t}) + \theta y_{1t} + 0.1 * \theta^2 y_{2t}$$

$$f_2^*(y_t) = \gamma \tan^{-1}(\alpha y_{2t}) + 0.1 * \theta^2 y_{1t} + \theta y_{2t}$$

$$f_3^*(y_t) = \gamma \tan^{-1}(\alpha y_{3t}) - 0.1 * \theta^2 y_{2t} + (\theta + 0.1 * \theta^2) y_{3t}$$

$$f_4^*(y_t) = \gamma \tan^{-1}(\alpha y_{4t}) + 0.1 * \theta^2 y_{3t} + (\theta - 0.1 * \theta^2) y_{4t}$$

$$f_5^*(y_t) = \gamma \tan^{-1}(\alpha y_{5t}) + 0.1 * \theta^2 y_{2t} + 0.1 * \theta^2 y_{4t} + \theta y_{5t}$$

and

$$u_{1t} = (\eta z_{1t} + z_{6t}^2) + f_1^*(y_t)$$

$$u_{2t} = (\eta_{22} z_{2t} + z_{6t}^2) + f_2^*(y_t)$$

$$u_{3t} = (\eta z_{3t} + z_{7t}^2) + f_3^*(y_t)$$

$$u_{4t} = (\eta_{44} z_{4t} + z_{7t}^2) + f_4^*(y_t)$$

$$u_{5t} = (\eta z_{5t} + z_{7t}^2) + f_5^*(y_t)$$

(c) Model (v), $n = 2$, $p = 6$

The model is:

$$f_1^*(y_t) = \gamma \tan^{-1}(\alpha y_{1t}) + (\theta + \theta^2)y_{1t} + \theta^2 y_{2t}$$

$$f_2^*(y_t) = \gamma \tan^{-1}(\alpha y_{2t}) - \theta^2 y_{1t} + (\theta + \theta^2)y_{2t}$$

and

$$u_{1t} = (\eta_{11}z_{1t} + (z_{3t}^2)^{\delta}) + f_1^*(y_t)$$

$$u_{2t} = (\eta_{22}z_{2t} + (z_{3t}^2)^{\delta}) + f_2^*(y_t)$$

(d) Model (vi), $n = 2$, $p = 4$

The model is:

$$f_1^*(y_t) = \gamma \tan^{-1}(\alpha y_{1t}) + (\theta + \theta^2)y_{1t} + \theta^2 y_{2t}$$

$$f_2^*(y_t) = \gamma \tan^{-1}(\alpha y_{2t}) - \theta^2 y_{1t} + (\theta * \theta^2)y_{2t}$$

and

$$u_{1t} = (\eta z_{1t} + z_{3t}^2) + f_1^*(y_t)$$

$$u_{2t} = (\eta z_{2t} + z_{3t}^2) + f_2^*(y_t)$$

REFERENCES

Amemiya, T. (1974), "The Nonlinear Two-stage Least Squares Estimators" Journal of Econometrics, 2, pp. 105-110.

__________ (1977), "The Maximum Likelihood and the Nonlinear Three-stage Least Squares Estimator in the General Nonlinear Simultaneous Equation Model", Econometrica, 45, pp. 955-968.

Bard, Y. (1970), "Comparison of Gradient Methods for the Solution of Nonlinear Parameter Estimation Problems", SIAM Journal of Numerical Analysis, 7, pp. 157-186.

Belsley, D.A. (1980), "On the Efficient Computation of the Nonlinear Full-information Maximum Likelihood Estimator", Journal of Econometrics, 14, pp. 203-225.

Berndt, E.K., Hall, B.H., Hall, R.E., and Hausman, J.A. (1974), "Estimation and Inference in Nonlinear Structural Models", Annals of Economic and Social Measurement, 3/4, pp. 653-666.

Brent, R.P. (1973), Algorithms for Minimization with Derivatives, Prentice-Hall Inc., Englewood Cliffs, N.J.

Broyden, C.G. (1970), "The Convergence of a Class of Double-rank Minimization Algorithms.. 2. The New Algorithm", Journal of the Institute of Mathematics and Applications, 6, pp. 222-231.

Brundy, J.M., and Jorgenson, D.W. (1974), "The Relative Efficiency of Instrumental Variables Estimators of Systems of Simultaneous Equations", Annals of Economic and Social Measurement, 3/4, pp. 679-699.

Byron, R.P. (1977), "Efficient Estimation and Inference in Large Econometric Systems", Econometrica, 45, pp. 1499-1515.

Chow, G.C. (1973), "On the Computation of Full-information Maximum Likelihood Estimates for Nonlinear Equation Systems", Review of Economics and Statistics, 55, pp. 104-109.

Cullum, J. (1972), "Modified Rank-One-No-Derivative Unconstrained Optimization Method (MRIND)", IBM Technical Disclosure Bulletin, 14, pp. 3732-3733.

Davidon, W.C. (1959), "Variable Metric Method for Minimization", A.E.C. R. & D. Report ANL-5990, Argonne National Laboratory.

____________ (1975), "Optimally Conditioned Optimization Algorithms Without Line Searches", Mathematical Programming, 9, pp. 1-30.

Dixon, L.W.C. (1972), "Nonlinear Optimization", English Universities Press, London.

____________ (1973), "Conjugate Directions Without Linear Searches", Journal of Mathematics and its Applications, 11, pp. 317-328.

Eisenpress, H., and Greenstadt, J. (1966), "The Estimation of Non-Linear Econometric Systems", Econometrica, 34, pp. 851-861.

Flanders, P.M., Hunt, D.J. Reddaway, and Parkinson, D. (1977), "Efficient High-Speed Computing with the Distributed Array Processor", paper presented at symposium on high-speed computer and algorithm organization, Illinois.

Fletcher, R., and Powell, M.J.D. (1963), "A Rapidly Convergent Descent Method for Minimization", The Computer Journal, 6, pp. 163-168.

Fletcher, R., and Reeves, C.M. (1964), "Function Minimization by Conjugate Gradients", The Computer Journal, 7, pp. 149-153.

Fletcher, R. (1970), "A New Approach to Variable Metric Algorithms", The Computer Journal, 13, pp. 317-322.

Gill, P.E., and Murray, W. (1972), "Quasi-Newton Methods for Unconstrained Optimization", Journal of the Institute of Mathematics and its Applications, 9, pp. 91-108.

Gill, P.E., Murray, W., and Pitfield, R.A. (1972), "The Implementation of Two Revised Quasi-Newton Algorithms for Unconstrained Optimization", NPL DNAC Report, No. 11.

Goldfarb, D. (1970), "A Family of Variable Metric Methods Derived by Variational Means", Mathematics of Computation, 24, pp. 23-26.

Goldfeld, S.M., and Quandt, R.E. (1972), Nonlinear Methods in Econometrics, North Holland, Amsterdam.

Gostick, R.W. (1979), "Software and Algorithms for the Distributed Array Processor", ICL Technical Journal, 1, pp. 116-135.

Gostick, R.W. (1981), "DAP Technical Reports", DAP Unit, Marketing Division, ICL.

Greenstadt, J. (1972), "A Quasi-Newton Method with no Derivatives", Mathematics of Computation, 26, pp. 145-166.

Hanson, J.W., Cariness, J.S., and Joseph, C. (1962), "Analytical Differentiation by Computer", Communication of the ACM, 5, pp. 349-355.

Hatanaka, M. (1978), "On the Efficient Estimation Methods for the Macro-economic Models Nonlinear in Variables", Journal of Econometrics, 8, pp. 323-356.

Hausman, J.A. (1975), "An Instrumental Variable Approach to Full Information Estimators for Linear and Certain Nonlinear Econometric Models", Econometrica, 43, pp. 727-738.

Hearn, A.C. (1976), "A new REDUCE Model for Algebraic Simplification", Proc. 1976 ACM Symposium on Symbolic and Algebraic Manipulation, ACM, N.Y., p. 46-54.

Hendry, D.F. (1971), "Maximum Likelihood Estimation of Systems of Simultaneous Regression Equations with Errors Geneiated by a Vector Autoregressive Process", International Economic Review, 12, pp. 257-271.

____________ (1974), "Stochastic Specification in an Aggregate Demand Model of the United Kingdom", Econometrica, 42, pp. 559-577.

____________ (1976), "The Structure of Simultaneous Equations Estimators", Journal of Econometrics, 4, pp. 51-88.

Hendry, D.F., and Tremayne, A.R. (1976), "Estimating Systems of Dynamic Reduced Form Equations with Vector Autoregressive Errors", International Economic Review, 17, pp. 463-471.

Hendry, D.F., and Srba, F. (1980), "AUTOREG: A Computer Library for Dynamic Econometric Models with Autoregressive Errors", Journal of Econometrics, 12, pp. 85-102.

Householder, A.S. (1964), The Thoery of Matrices in Numerical Analysis, Blaisdell Publishing Co., New York.

ICL (1979), DAP: APAL Language.

ICL (1981), DAP: FORTRAN Language.

Jacoby, S.L.S., Kowalik, J.S., and Pizzo, J.T. (1972), Iterative Methods for Nonlinear Optimization Problems, Prentice Hall, Englewood Cliffs, NJ.

Kendall, M.G., and Stuart, A. (1961), The Advanced Theory of Statistics, Vol. 2, Chapter 18, pp. 37-77, Charles Griffin & Co. Ltd., London.

Knuth, E. (1969), The Art of Computer Programming, Vol. 1, Addison-Wesley Publishing Co., Reading, Mass.

Kowalik, J., and Osborne, M.R. (1968), Methods for Unconstrained Optimization Problems, Elsevier Publishing Co. Inc., N.Y.

Lesk, A.M. (1967), "Dynamic Computation of Derivations", Communications of the ACM, 10, pp. 571-572.

MACSYMA Reference Manual, The Marhlab Group, Laboratory for Computer Science, MIT, Version 9, 1977.

Mifflin, R. (1974), "A Superlinearly Convergent Algorithm of Minimization Without Evaluating Derivatives", Report No. 65, Administrative Sciences, Yale University.

Murray, W. (1972), Numerical Methods for Unconstrained Optimization, Academic Press, London.

Parkinson, D. (June 1976), "Computer by the Thousand", New Scientist, 17, pp. 626-627.

____________ (Nov. 1976), "Technical Description of the Distributed Array Processor", ICL Report AP2.

____________ (Nov. 1977), An Introduction to Array Processors, Systems International.

____________ (1980), "Practical Parallel Processors and Their Uses", Technical Report, Queen Mary College DAP Support Unit.

Powell, M.J.D. (1964), "An Efficient Method of Finding the Minimum of a Function of Several Variables Without Calculating Derivatives", The Computer Journal, 7, pp. 155-162.

Powell, M.J.D. (1971), "Recent Advances in Unconstrained Optimization", Mathematical Programming, 1, pp. 26-57.

_____________ (1977), "Restart Procedures for the Conjugate Gradient Method", Mathematical Programming, 12, pp. 241-254.

REDUCE Reference Manual, University of Utah Computer Physics Group.

Sammet, J.E. (1966), "Survey of Formula Manipulation", Communications of the ACM, 9, pp. 555-569.

Sargan, J.D., and Sylwestrowicz, J.D. (1976), "A Comparison of Alternative Methods of Numerical Optimization in Estimating Simultaneous Equation Econometric Models", SSRC Discussion Paper.

Sargan, J.D., and Chong, Y.Y. (1980), "A General Differentiation Program With Particular Application to the Estimation of Econometric Models", SSRC Discussion Paper.

Smith, P.J. (1965), "Symbolic Derivatives Without List Processing, Subroutines, or Recursion", Communications of the ACM, 8, pp. 494-496.

Stewart, G.W. (1967), "Modification of Davidon's Minimization Method to Accept Difference Approximations to Derivatives", Journal of the Association of Computer Machinery, 14, pp. 72-83.

Theil, H. (1971), Principles of Econometrics, Section 8.4, pp. 384-391, John Wiley & Sons, New York.

Thurber, K.J., and Wald, L.D. (1975), "Associative and Parallel Processors", Computing Surveys, 7, pp. 215-255.

Wessgert, R.E. (1964), "A Simple Automatic Derivative Evaluation Program", Communications of the ACM, 7, pp. 463-464.

Wolfe, M.A. (1978), Numerical Methods for Unconstrained Optimization, Van Nostrand Reinhold Co., New York.