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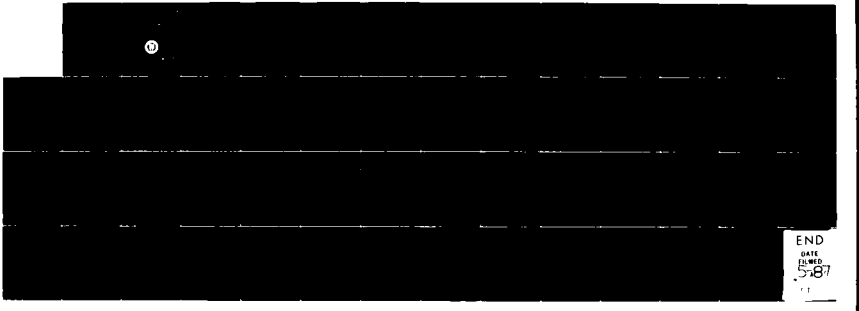

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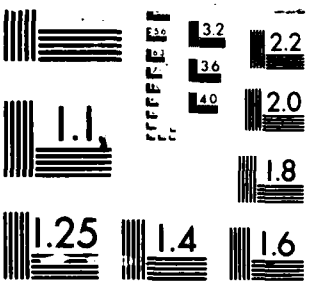

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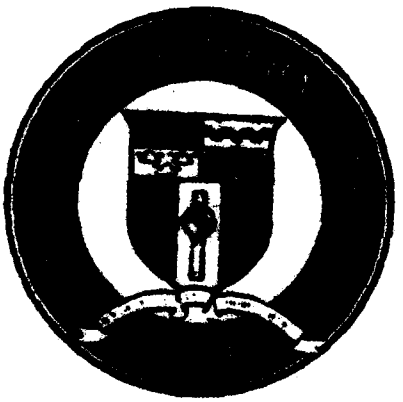
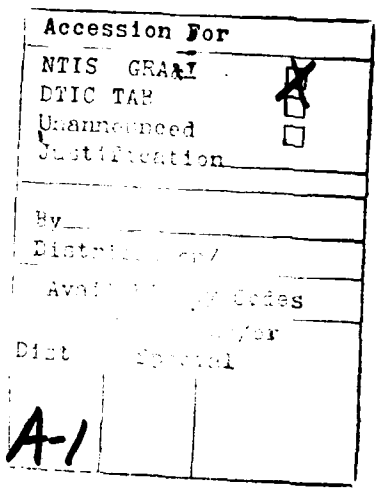


# A FAMILY OF ALGORITHMS FOR THE ESTIMATION OF THE PARAMETERS OF THE STABLE LAWS AND THE PARAMETERS OF ATTRACTING STABLE LAWS

by

T. A. Delehanty
and
A. S. Paulson



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## DESCRIPTION AND PURPOSE

Potential application of the stable laws has long been hindered by the unavailability of generally available, well-documented algorithms. This paper removes this deficiency by presenting an algorithm for estimation of stable law parameters, with the goal of facilitating the application of stable laws in modeling and inference frameworks. The stable laws have steadily increased in importance to the statistical community since the paper of Mandelbrot (1963). Their role as the only laws possessing domains of attraction makes the stable laws an appealing probabilistic model, and they are capable of modeling a wide range of skewness, heavy tailedness, and central peakedness. Procedures for estimation of stable law parameters have been described by Mandelbrot (1963), DuMouchel (1971), Fama and Roll (1971), Paulson, Holcomb, and Leitch (1975), Koutrouvelis (1980,1981), Feuerverger and McDunnough (1981a,1981b), and Brockwell and Brown (1981). Because of the intractability of stable densities, attention has centered in recent years on Fourier-based procedures, using the empirical characteristic function. Such procedures should have an adaptive nature (Paulson, Holcomb, and Leitch, 1975; Paulson, Delehanty, and Brothers, 1982; Paulson and Delehanty, 1982).

This document ~~We~~ presents an iterative and adaptive algorithm for joint estimation of stable law parameters, using the empirical characteristic function. The algorithm is flexible in that either of two procedures may be selected, and subsets of the parameters may be allowed to vary freely, with others constrained or held constant. The statistical rationale for the procedures is described in the companion paper by Paulson and Delehanty (1982). The algorithm may also be used to provide informal estimates of the parameters

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of the stable law to which a sample distribution is attracted.

## THEORY AND NOTATION

Nondegenerate stable random variables X may be defined by the characteristic function

$$\phi(u) = E(\exp iuX) = \exp\{iu\mu - |\sigma u|^{\alpha}(1+i\beta\ \mathrm{sgn}(u)\ \chi(u,\alpha))\}, \tag{1}$$

where $i^2 = -1$, $0 < \alpha \leq 2, |\beta| \leq 1$, $\sigma > 0$, and

$$\chi(u,\alpha) = \begin{cases} \tan\frac{\pi\alpha}{2}, & \alpha \neq 1 \\ \frac{2}{\pi}\log|u|, & \alpha = 1. \end{cases} \tag{2}$$

Here $\alpha$, the characteristic exponent, is a measure of heavy tailedness and central peakedness, $\beta$ is a skewness measure, $\sigma$ is a scale parameter, and $\mu$ is a location parameter unless ($\alpha=1$, $\beta\neq 0$), when the function of location parameter is assumed by $\mu + \frac{2}{\pi}\beta\sigma\log\sigma$. The only stable laws whose densities are expressible in closed form are the Gaussian ($\alpha=2$, $\beta=0$), the Cauchy ($\alpha=1, \beta=0$), and the reciprocal of a $\chi^2$ variate on one degree of freedom ($\alpha=\frac{1}{2}, \beta=-1$).

Let $X_1,\ldots,X_n$ be a stable random sample. The empirical characteristic function is

$$\phi_n(u) = n^{-1}\sum_{j=1}^{n}\exp(iuX_j). \tag{3}$$

Let $\psi(u) = \mathrm{Re}\ \phi(u) + \mathrm{Im}\ \phi(u)$, $\psi_n(u) = \mathrm{Re}\ \phi_n(u) + \mathrm{Im}\ \phi_n(u)$. Estimators interior to the parameter space can be viewed as zeros of the systems

Formulation A

$$\sum_{j=1}^{q}\frac{\partial\psi(u_j)}{\partial\theta}(\psi(u_j) - \psi_n(u_j))w_j = 0, \tag{4}$$

or

Formulation B

$$\sum_{j=1}^{q} \sum_{k=1}^{q} \frac{\partial \psi(u_j)}{\partial \theta} K^{jk} (\psi(u_k) - \psi_n(u_k)) w_j w_k = 0, \qquad (5)$$

for $\theta = \alpha, \beta, \sigma, \mu$. The grid $\{u_j | j=1,\ldots,q\}$ is symmetric about zero but does not include the origin, and $K^{jk}$ denotes the j,k element of the inverse matrix $(K_{jk})^{-1}$, where

$$K_{jk} = n \operatorname{cov}(\psi_n(u_j), \psi_n(u_k))$$

$$= \operatorname{Re} \phi(u_j - u_k) + \operatorname{Im} \phi(u_j + u_k) - \psi(u_j)\, \psi(u_k). \qquad (6)$$

The weights $\{w_j | j=1,\ldots,q\}$ also depend on the parameters $\alpha, \beta, \sigma, \mu$, and are described in the Numerical Method section. Both Formulations A and B represent modified, weighted $\chi^2$ minimum procedures, corresponding to the respective objective functions

$$\text{A:} \qquad S_n = \sum_{j=1}^{q} (\psi(u_j) - \psi_n(u_j))^2 w_j, \qquad (7)$$

$$\text{B:} \qquad Q_n = \sum_{j=1}^{q} \sum_{k=1}^{q} (\psi(u_j) - \psi_n(u_j))\, w_j\, K^{jk}\, w_k (\psi(u_k) - \psi_n(u_k)). \qquad (8)$$

The following points are critical for practical application:

1) The shapes of $\psi$ and $\psi_n$ are highly dependent on location and scale parameters, and so should be standardized;

2) The estimators are improved by making the gridpoints and weights depend on $\alpha$ and $\beta$;

3) Since the procedures are adaptive ($\{u_j\}$,$\{w_j\}$ and $\{K_{jk}\}$ depend on unknown parameters), algorithms must be iterative;

4) Since $\alpha$, $\beta$ and $\sigma$ are always constrained, each iteration involves solution of a nonlinear optimization problem with variable bound constraints.

Our procedures may therefore be summarized as follows, where a tilde indicates estimators, their values, or adaptively standardized quantities.

Begin with initial guesses for the parameters. At each iteration, compute and save $\{u_j\}$, $\{w_j\}$, possibly $\{K^{jk}\}$, and standardized empirical characteristic function values $\{\tilde{\psi}_n(u_j)\}$, based on the latest $(\tilde{\alpha},\tilde{\beta})$. The objective $S_n$ or $Q_n$ is then minimized (an "optimization subproblem"), and cumulative location and scale estimates $(\tilde{\ell},\tilde{s})$ are updated. Iteration stops when values of $\sigma$ and $\mu$ minimizing $S_n$ or $Q_n$ are acceptably close to unity and zero, respectively.

Estimators whose values are not on a bound are asymptotically multivariate Gaussian distributed. The asymptotic covariance matrices $\underset{\sim}{\Sigma}$ of the estimators are derived in Paulson and Delehanty (1982). The basic formula is

$$\underset{\sim}{\Sigma}_i = \underset{\sim}{H}_i^{-1} \underset{\sim}{V}_i \underset{\sim}{H}_i^{-1}, \qquad i = A,B. \tag{9}$$

There are two particularly appealing ways to approximate $\underset{\sim}{\Sigma}$. In "approximation (i)", expectations are approximated from the data: $\underset{\sim}{H}$ is computed by differencing the objective at the final optimum, and

$$\underset{\sim}{V}_A = 4\underset{\sim}{D}^T\tilde{\underset{\sim}{K}}\underset{\sim}{D}, \tag{10}$$

$$\underset{\sim}{V}_B = 4\underset{\sim}{D}^T\underset{\sim}{K}^{-1}\tilde{\underset{\sim}{K}}^{(w)}\underset{\sim}{K}^{-1}\underset{\sim}{D}. \tag{11}$$

Here

$$D_{j\theta} = \frac{\partial\tilde{\psi}(u_j)}{\partial\theta}\, w_j, \tag{12}$$

$\theta$ ranging over the parameters free of bounds,

$$\tilde{K}_{jk} = n^{-1} \sum_{m=1}^{n} (\tilde{\psi}(u_j) - \cos u_j \tilde{x}_m - \sin u_j \tilde{x}_m)(\tilde{\psi}(u_k) - \cos u_k \tilde{x}_m - \sin u_k \tilde{x}_m), \tag{13}$$

and

$$\tilde{\underset{\sim}{K}}^{(w)}_{jk} = \tilde{\underset{\sim}{K}}_{jk}\, w_j w_k. \tag{14}$$

By location and scale invariance, $(\tilde{\sigma},\tilde{\mu})$ are set to (1,0) during these computations, and $\underset{\sim}{\Sigma}$ scaled. In "approximation (ii)", expectations are calculated analytically, so $\underset{\sim}{K}$ replaces $\tilde{\underset{\sim}{K}}$ in (10), (11), and (14), and factors of 2 are omitted. The expected Hessian has elements

$$H_{A\theta\theta'} = \sum_{j=1}^{q} \frac{\partial\tilde{\psi}(u_j)}{\partial\theta} \frac{\partial\tilde{\psi}(u_j)}{\partial\theta'} w_j, \tag{15}$$

$$H_{B\theta\theta'} = \underset{\sim}{D}^T \underset{\sim}{K}^{-1} \underset{\sim}{D},$$

where $\theta$ and $\theta'$ range over free parameters.

To analyze domains of attraction, we use what we refer to as the k-sum procedure. If k is a positive integer, the power

$$\phi_n^k(u) = n^{-k} \sum_{j_1=1}^{n} \cdots \sum_{j_k=1}^{n} \exp(iu(x_{j_1} + \cdots + x_{j_k})) \tag{16}$$

is the characteristic function corresponding to the $k^{th}$ convolution power of the empirical distribution function $F_n(x)$, and can be interpreted as empirical characteristic function of all possible k-sums $\{x_{j_1} + \cdots + x_{j_k}\}$, sampling with replacement from $F_n(x)$. We add real and imaginary parts and standardize, giving $\tilde{\psi}_n^k(u)$, say, and estimate $(\tilde{\alpha}_k, \tilde{\beta}_k, \tilde{\sigma}_k, \tilde{\mu}_k)$ for different values of k. If the sample distribution is

attracted to a stable law with parameters $(\alpha,\beta,\sigma,\mu)$, the sequence of normalized estimators $(\tilde{\alpha}_k, \tilde{\beta}_k, \tilde{\sigma}_k/k^{1/\tilde{\alpha}_k}, \tilde{\mu}_k/k)$, for reasonable values of k, should approach $(\alpha,\beta,\sigma,\mu)$. In particular, a rapid rise in $\{\tilde{\alpha}_k\}$ may indicate that a stable model is not appropriate, a possible alternative being a mixture of finite variance components with differing scale parameters.

The k-sum procedure can thus be used in a sensitivity analysis, to examine how well the data support the stability assumption. Other possible tools for sensitivity analysis are varying the mechanism (to be described below) underlying the weights $\{w_j\}$, and comparing approximations (i) and (ii) of the estimated asymptotic covariance matrix, provided n is large enough for approximation (i) to be accurate.

## NUMERICAL METHOD

The main computational task required is solution of bound-constrained nonlinear optimization problems. Although Formulations A and B lead to nonlinear least squares problems, current algorithms for nonlinear least squares do not allow constraints (Hiebert, 1981). Numerical Algorithms Group (NAG) subroutine E04KBF (NAG, 1981) is used for optimization. E04KBF is a quasi-Newton procedure, requiring an objective function and analytical first partial derivatives. It is substantially faster than the gradient projection routine used by Paulson, Holcomb and Leitch (1975), although the latter is very reliable. The other complicated numerical procedure required is inversion of a positive definite symmetric matrix ($\underset{\sim}{K}$, $\underset{\sim}{H}$ or $\tilde{\underset{\sim}{H}}$), for which NAG subroutine F01ABF is used. Various NAG utility procedures are also used, see Auxiliary Algorithms. The use of NAG

procedures inhibits transportability in that the algorithm, as presented, is only usable at installations having the NAG Library. However, listings of rapid, high-quality algorithms for constrained optimization have not appeared in the literature (see Chambers, 1977, pp. 159-160; the situation described there has not improved). Given that E04KBF is used, reliance on additional NAG Library procedures is expedient.

We require a minimum of q=20 gridpoints $\{u_j\}$, and prefer q=20 or 40, since they are reasonable values in practice, and have been tested extensively. Only the positive gridpoints are explicitly required, due to symmetry of the grid and the Hermitian property of characteristic functions. They are computed as follows: An endpoint U is chosen as 3, $\tilde{\alpha} \geq 1.8$; 3.3, $1.8 > \tilde{\alpha} \geq 1.7$; 3.6, $1.7 > \tilde{\alpha} > 1$; 5, $\tilde{\alpha}=1$; 4, $1 > \tilde{\alpha} \geq .9$; 5, $.9 > \tilde{\alpha} \geq .8$; 7, $.8 > \tilde{\alpha} \geq .6$; 10, $\tilde{\alpha} < .6$. An inner number I of points is selected close to the origin: I=2 if q<30 and 3 if q≥30, 1 being subtracted if $\tilde{\alpha} \leq .5$. The inner I points are spaced as follows: if $\tilde{\alpha}>1$, ½ the "α-optimal" values of Feuerverger and McDunnough (1981b) for the nearest (larger) α are used; if $\tilde{\alpha} \leq 1$, the first I points giving q/2 equal increments of $\log (u + \alpha^{*3})$ between 0 and U are multiplied by ½ $\alpha^{*2}$ ($\alpha^{*} = \max(\tilde{\alpha}, .3)$). The remaining points are logarithmically spaced out to U: if $\tilde{\alpha}>1$, the function $\log (1 + u/2)$ is used, and if $\tilde{\alpha} \leq 1$, $\log(u + \alpha^{*3})$ is used. This rather complicated ad hoc scheme was developed through graphical inspection of $\tilde{\psi}(u)$ and $\tilde{\psi}_n(u)$, comparisons of asymptotic efficiencies, and parameter estimation for real and simulated data. No claims of optimality are made, but the scheme provides high efficiencies if efficiency is preferred, or good matches between $\tilde{\psi}$ and $\tilde{\psi}_n$ if curve fitting is preferred. The point of stratified and logarithmic spacing is

to emphasize u values near the origin. Details when $\tilde{\alpha} \leq 1$ reflect the fact that $\psi(u)$ has a sharp cusp near the origin, but decays slowly. The stepwise nature of the scheme is not deemed a serious drawback.

The weights $\{w_j\}$ are computed as follows:

Under Formulation A,

$$w_j = \frac{|\phi(u_j)|^{2\lambda}}{K_\tau(u_j,u_j)} = \frac{\exp(-2\lambda|u_j|^\alpha)}{K_\tau(u_j,u_j)} \quad , \tag{17}$$

and under Formulation B,

$$w_j = |\phi(u_j)|^\lambda = \exp(-\lambda|u_j|^\alpha), \tag{18}$$

where $\lambda$ and $\tau$ are supplied by the user, $0 \leq \tau \leq 1$,

$$K_\tau(u,u) = 1 + \tau(\text{Im } \tilde{\phi}(2u) - \tilde{\psi}^2(u)), \tag{19}$$

and $\lambda$ is recommended nonnegative. Rationale for these weights, and some corresponding asymptotic efficiencies, are in Paulson and Delehanty (1982). We recommend $\tau=1$ under Formulation A. Under Formulation B, it is convenient to let $\tau \geq 0$ represent a fraction of the average diagonal element by which to inflate K, giving a matrix we shall call A. We have only found this inflation necessary if $\tilde{\alpha}$ is very close to two, when $\tau = 0.01$ suffices.

To use the quantity $\lambda$ as a tool for sensitivity analysis, we interpret it as a damping factor, lessening the effects of noise in $\tilde{\psi}_n(u)$ for larger $|u|$. If the data are truly stable and the sample size is fairly large (say 150 or more), estimates should change little as $\lambda$ varies, say, from 0 to 1. Large discrepancies in the estimates for different values of $\lambda$ indicate problems with the data or the stable assumption or both. It may not be easy to isolate the difficulty but further study is

definitely required.

For the k-sum procedure, k>1, the situation regarding gridpoints and weights changes. Tests so far indicate that when $\tilde{\alpha}>1$, Formulation A, with gridpoints equispaced from 0 to U, gives better results than "efficient configurations" used for k=1. Reasons for this are unclear. A possible explanation is that when $\tilde{\alpha}>1$ and k>1, $\tilde{\psi}_n^k(u)$ is so smooth that estimation is practically equivalent to deterministic curve fitting, and implicit or explicit emphasis on gridpoints near the origin neglects important curvature for large $|u|$. Accordingly, when k>1 and $\tilde{\alpha}>1$, we equispace gridpoints and set all weights to 1. When $\tilde{\alpha}\leq 1$, $\tilde{\psi}_n^k(u)$ has a sharp cusp near the origin and remains a jagged curve as k increases, due to the presence of very large observations. In this situation, we set all weights to 1 and use basically the same gridpoint scheme as when k=1, omitting only multiplication of the inner points by $\alpha^{*2}/4$. In either case, Formulation A is recommended.

An important question is how large k may be taken. Equation (16) suggests that we cannot expect to take k arbitrarily large. There seems to be a tendency for $\tilde{\alpha}$ to increase and $\tilde{\beta}$ to drift if k is too large, though this may be partially due to suboptimal gridpoints or weighting. It appears that when n is large, say 500 or more, k may safely be taken up to 20. Care is required for smaller n, and when $\alpha$ is small or very near two.

Implicit standardization is carried out as follows. Let k be a positive integer, and $(\tilde{\ell},\tilde{s})$ cumulative location and scale estimates. Then

$$\tilde{\psi}_n^k(u_j) = \rho_{jk}(\cos \gamma_{jk} + \sin \gamma_{jk}), \tag{20}$$

where

$$\rho_{jk} = |\phi_n(u_j/\tilde{s})|^k \tag{21}$$

and

$$\gamma_{jk} = k \arg\phi_n(u_j/\tilde{s}) - \tilde{\ell}u_j/\tilde{s}. \tag{22}$$

No problems of principal values arise, and complex arithmetic is not used. The FORTRAN mathematical library function ATAN2 computes arguments.

The estimator $\tilde{\alpha}$ may be bounded in (closed) subintervals of $[\delta,1-\varepsilon]$, $[1,1]$, or $[1+\varepsilon,2]$ unless $\tilde{\beta}$ is fixed at 0, when $[\delta,2]$ is possible ($\delta$ and $\varepsilon$ are small positive numbers), while $\tilde{\beta}$ may be bounded in subintervals of $[-1,1]$. Estimators $\tilde{\sigma}$ and $\tilde{\mu}$ may be constrained arbitrarily in$[\delta,\infty)$ and $(-\infty,\infty)$, respectively, unless $\tilde{\alpha}$ is fixed at 1 and $\tilde{\beta}$ is not fixed at 0, when $\tilde{\mu}$ cannot be constrained. Bounds on $\sigma$ and $\mu$ are internally set for use in subproblems. These bounds must be wide enough to allow the "true values" to be found, but narrow enough to deter straying into undesirable regions, particularly $\sigma\to\infty$, $|\mu|\to\infty$. The ad hoc bounds of $[-5,5]$ for $\mu$ and $[0.2,5]$ for $\sigma$ work well in practice. If $\tilde{\sigma}$ or $\tilde{\mu}$ are initially constrained, their internal bounds are adaptively modified, see the Algorithm for description.

Initial guesses for the parameters are required. We do not find their specification particularly important, provided $\tilde{\alpha}$ is on the correct side of 1 in the nonsymmetric case. We have used the median and semi-interquartile range as guesses for $\tilde{\mu}$ and $\tilde{\sigma}$, and averages of upper and lower bounds for $\tilde{\alpha}$ and $\tilde{\beta}$. If $\tilde{\alpha}$ is anticipated less than 1.2, say, it is

worthwhile to put more effort into initial guesses, since fewer iterations will be required (the semi-interquartile range will overestimate $\sigma$, and if $\alpha$ is near but different from 1, the median is nearer $\mu - \frac{2}{\pi}\beta\sigma\log\sigma$ than $\mu$).

Convergence is judged by a tolerance on subproblem solutions, $\max(|\sigma^{(m)}-1|, |\mu^{(m)}|)$, (or $\max(|\alpha^{(m)} - \alpha^{(m-1)}|, |\beta^{(m)} - \beta^{(m-1)}|)$ if $\tilde{\sigma}$ and $\tilde{\mu}$ are fixed), with a maximum allowable number of iterations. Attainable tolerances depend on n, but more strongly on the underlying parameters. If $\tilde{\alpha}$ is near two, $\tilde{\psi}_n$ is very smooth and stringent tolerances such as $10^{-6}$ may be attained. If $\tilde{\alpha}\leq 1.2$, $\tilde{\psi}_n$ has many small oscillations due to large observations, and, especially for smaller samples, it may be preferable to terminate after a fixed number of iterations. Good estimates are generally obtained within five iterations, fewer if initial guesses are good; if stringent tolerances are required, or for difficult problems (skewed distributions with $0.9\leq\alpha\leq 1.1$) more may be required. Convergence is typically slower under Formulation B, since the weighting mechanism is more complicated.

Approximation of asymptotic covariance matrices requires little description. We note that for approximation (i) and the q values we use, it is faster to define a vector

$$\delta_j^T = (\tilde{\psi}(u_1) - \cos u_1\tilde{x}_j - \sin u_1\tilde{x}_j, \cdots, \tilde{\psi}(u_q) - \cos u_q\tilde{x}_j - \sin u_q\tilde{x}_j), \tag{23}$$

and cumulate

$$\tilde{V} = 4n^{-1}\sum_{j=1}^{n}(\underline{D}^T\delta_j)(\underline{D}^T\delta_j)^T \tag{24}$$

under Formulation A, or

$$\tilde{V} = 4n^{-1} \sum_{j=1}^{n} (D^T A^{-1} \delta_j)(D^T A^{-1} \delta_j)^T \qquad (25)$$

under Formulation B, than to cumulate $\tilde{K}$. The matrix $D$ is computed by the function/gradient subroutine. E04KBF returns an approximate Hessian, which could conceivably be used for $\tilde{H}$ in approximation (i). Rather often, however, E04KBF will terminate with its failure indicator set to 3 and the Hessian set to the identity matrix, even though the optimum may be reliable. It is therefore simpler to compute $\tilde{H}$ by differencing. The following procedures is used: Set an initial Hessian to 0, and the steplength to $10^{-3}$. Successively divide the steplength by $\sqrt{10}$ and approximate the Hessian by differencing; three-point differencing for the diagonal, and four-point for off-diagonal elements. Compare elements of successive approximations by maximum relative or absolute differences, according as the element of the latest approximation exceeds 1 in absolute value or not. A tolerance of $10^{-6}$ is used for this convergence criterion. If convergence has not occurred with a steplength of $10^{-5}$, the result with steplength $10^{-4}$ is used.

Approximation (i) of the asymptotic covariance matrix is rather expensive to compute. It should not be computed for smaller sample sizes, as it implicitly involves estimation of $\frac{1}{2}q(\frac{1}{2}q+1)$ covariances.

Following is an informal description, in Algorithm form, of the basic routine STABLE. Approximate asymptotic covariance matrices may also be computed, but this presents no logical difficulties, so is omitted.

Algorithm

Produces estimates $(\tilde{\alpha},\tilde{\beta},\tilde{\sigma},\tilde{\mu})$ for k-sums (k≥1), based on a sample $(x_1,\ldots,x_n)$.

Input parameters: k, n, $\{x_j\}$, q, λ, τ, Formulation (A or B), convergence tolerance ε, maximum number M of iterations, and flags whether $\tilde{\sigma}$ and $\tilde{\mu}$ are constrained.

Input/output parameters: $(\tilde{\alpha},\tilde{\beta},\tilde{\sigma},\tilde{\mu})$ are initial guesses on entry and estimates on exit, $(\alpha_L,\beta_L,\sigma_L,\mu_L)$ and $(\alpha_u,\beta_u,\sigma_u,\mu_u)$ are lower bounds. The $(\sigma,\mu)$ bounds are changed, but restored on exit. In the special case where $\tilde{\alpha}$ is fixed at 1, $\tilde{\mu}$, on entry, is the initial guess for location $\mu + \frac{2}{\pi}\beta\sigma\log\sigma$.

Auxiliary quantities $\tilde{\ell}$ and $\tilde{s}$ are cumulative location and scale estimates. Entry values of $(\sigma_L,\sigma_u,\mu_L,\mu_u)$ are stored in $(b_1,b_2,b_3,b_4)$. On entry and exit, $(\tilde{\sigma},\tilde{\mu},\sigma_L,\mu_L,\sigma_u,\mu_u)$ are normalized.

S1 [Initialize.]

Set $\tilde{\ell} \leftarrow k\tilde{\mu}$, $\tilde{s} \leftarrow k^{1/\tilde{\alpha}}\,\tilde{\sigma}$, $m \leftarrow 0$.

Save $(b_1,b_2,b_3,b_4) \leftarrow (\sigma_L,\sigma_u,\mu_L,\mu_u)$.

if $\tilde{\mu}$ is unconstrained then set $\mu_L \leftarrow -5$, $\mu_u \leftarrow 5$;

else if $\tilde{\mu}$ is fixed then set $\mu_L \leftarrow \mu_u \leftarrow 0$;

else set $\mu_L \leftarrow k\mu_L$, $\mu_u \leftarrow k\mu_u$.

if $\tilde{\sigma}$ is unconstrained then set $\sigma_L \leftarrow 0.2$, $\sigma_u \leftarrow 5$;

else if $\tilde{\sigma}$ is fixed then set $\sigma_L \leftarrow \sigma_u \leftarrow 1$;

else set $\sigma_L \leftarrow k^{1/\tilde{\alpha}}\,\sigma_L$, $\sigma_u \leftarrow k^{1/\tilde{\alpha}}\,\sigma_u$.

S2 [Looping point for iteration; save adaptive quantities for subproblem.]

Increment $m \leftarrow m + 1$.

Save $\tilde{\alpha}^{(m-1)} \leftarrow \tilde{\alpha}$, $\tilde{\beta}^{(m-1)} \leftarrow \tilde{\beta}$.

if $\tilde{\sigma}$ is constrained but not fixed then set $\sigma_L \leftarrow \max(0.2, b_1/\tilde{s})$,

$\sigma_u \leftarrow \min(5, b_2/\tilde{s})$.

if $\tilde{\mu}$ is constrained but not fixed then set $\mu_L \leftarrow \max(-5, (b_3-\tilde{\ell})/\tilde{s})$,

$\mu_u \leftarrow \min(5, (b_4-\tilde{\ell})/\tilde{s})$.

Set $\tilde{\sigma} \leftarrow 1$, $\tilde{\mu} \leftarrow 0$.

Compute and save positive gridpoints $\{u_j \mid j = q/2+1, \ldots, q\}$,

weights $\{w_j \mid j=1,\ldots,q\}$, and standardized empirical characteristic function values $\{\tilde{\psi}_n^k(u_j) \mid j=1,\ldots,q\}$.

if Formulation B then compute and invert A.

S3 [Subproblem.]

Solve the optimization problem

$$\min \sum_{j=1}^{q} (\psi(u_j) - \tilde{\psi}_n^k(u_j))^2 w_j \qquad \text{(Formulation A)}$$

or

$$\min \sum_{i=1}^{q} \sum_{j=1}^{q} w_i(\psi(u_i) - \tilde{\psi}_n^k(u_i))\, A^{ij} (\psi(u_j) - \tilde{\psi}_n^k(u_j)) w_i \quad \text{(Formulation B)},$$

yielding new $(\tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}, \tilde{\mu})$.

S4 [Update and test convergence.]

Set $\tilde{\ell} \leftarrow \tilde{\ell} + \tilde{s}\,\tilde{\sigma}$.

if $\tilde{\alpha}=1$ then set $\tilde{\ell} \leftarrow \tilde{\ell} + \frac{2}{\pi}\,\tilde{s}\,\tilde{\beta}\,\tilde{\sigma}\log\tilde{\sigma}$.

Set $\tilde{s} \leftarrow \tilde{s}\,\tilde{\sigma}$.

<u>if</u> $\tilde{\sigma}$ and $\tilde{\mu}$ are fixed <u>then</u> error $\leftarrow \max\left(|\tilde{\alpha}-\tilde{\alpha}^{(m-1)}|,\ |\tilde{\beta}-\tilde{\beta}^{(m-1)}|\right)$;

<u>else</u> error $\leftarrow \max\left(|\tilde{\sigma}-1|, |\tilde{\mu}|\right)$.

<u>if</u> error $\geq \varepsilon$ and $m<M$ <u>then</u> go to <u>S2</u>.

<u>S5</u> [Final estimates.]

Set $(\sigma_L,\sigma_u,\mu_L,\mu_u) \leftarrow (b_1,b_2,b_3,b_4)$.

<u>if</u> $\tilde{\alpha}=1$ <u>then</u> set $\tilde{\ell} \leftarrow \tilde{\ell} - \frac{2}{\pi}\,\tilde{\beta}\,\tilde{s}\log\tilde{s}$.

Set $\tilde{\mu}\leftarrow\tilde{\ell}/k$, $\tilde{\sigma}\leftarrow\tilde{s}/k^{1/\tilde{\alpha}}$.

## STRUCTURE

```
SUBROUTINE STABLE (X,N,MODE,KSUM,XLAM,TAU,NPTS,TOL,MAXIT,XL,XB,XH,NPAR,
ISCLBD,LOCBND,ICOV,VCV1,VCV2,WORK,LWORK,IWORK,LIWORK,IFAULT)
```

Formal parameters

| | | | |
|---|---|---|---|
| X | Real array (N) | input: | sample |
| N | Integer | input: | sample size |
| MODE | Integer | input: | formulation; if zero, then Formulation B is used, else Formulation A |
| KSUM | Integer | input: | convolution power k |
| XLAM | Real | input: | $\lambda$ |
| TAU | Real | input: | $\tau$ |
| NPTS | Integer | input: | q |
| TOL | Real | input: | convergence tolerance |
| MAXIT | Integer | input: | maximum allowable number of iterations |
| XL | Real array (NPAR) | input: | lower bounds for parameters ($\alpha,\beta,\sigma,\mu$); the third and fourth elements change during execution |
| | | output: | input values are restored |
| XH | Real array (NPAR) | input: | upper bounds for parameters; the third and fourth elements change during execution |
| | | output: | input values are restored |
| NPAR | Integer | input: | number of parameters (4) |
| ISCLBD | Integer | input: | flag if $\tilde{\sigma}$ is constrained: if negative, $\tilde{\sigma}$ is fixed at XB(3); if zero, $\tilde{\sigma}$ is free to vary and initial values of XL(3) and XH(3) are irrelevant; if positive, $\tilde{\sigma}$ is constrained in [XL(3),XH(3)] |

| | | | |
|---|---|---|---|
| LOCBND | Integer | input: | flag if $\tilde{\mu}$ is constrained: if negative, $\tilde{\mu}$ is fixed at XB(4); if zero, $\tilde{\mu}$ is free to vary and initial values of XL(4) and XH(4) are irrelevant; if positive, $\tilde{\mu}$ is constrained in [XL(4),XH(4)] |
| ICOV | Integer | input: | flag for computation of covariance matrices: if negative, neither approximation (i) nor (ii) is computed; if zero, both approximations are computed; if positive, only approximation (ii) is computed |
| VCV1 | Real array(NPAR,NPAR) | output: | covariance matrix approximation (i) if requested; the strict lower triangle contains correlations, the upper triangle contains covariances (times n); if a parameter is on a bound, the corresponding elements are zero |
| VCV2 | Real array(NPAR,NPAR) | output: | covariance matrix approximation (ii) if requested; the strict lower triangle contains correlations, the upper triangle covariances (times n); if a parameter is on a bound, the corresponding elements are zero |
| WORK | Real array (LWORK) | workspace: | |
| | | output: | some elements may be of interest on output (see Restrictions) |
| LWORK | Integer | input: | |
| IWORK | Integer array(LIWORK) | workspace: | |
| | | output: | some elements may be of interest on output (see Restrictions) |
| LIWORK | Integer | input: | |
| IVNIT | Integer | input: | if positive, unit number for output (see Additional Comments); if zero or negative, no output is produced |
| IFAULT | Integer | output: | failure indicator |

Failure indicators

IFAULT = 0 indicates success. Nonzero values of IFAULT are due to two types of errors. The first type is input errors, detected in STABLE; IFAULT will be

1 if MAXIT≤0;

2 if N<50 (see Restrictions);

3 if KSUM ≤ 0;

4 if $\tau<0$ or $\tau>1$ and MODE≠0;

5 if NPTS<20 or mod(NPTS,2)≠0;

6 if TOL≤0;

7 if NPAR≠4;

8 if insufficient workspace was allotted (see Restrictions);

9 if improper bounds were supplied. The following conditions cause this failure:
XL(i)>XB(i) or XL(i)>XH(i) or XB(i)>XH(i), i=1,2
XL(1)≤0 or XH(1)>2
XL(1)<-1 or XH(1)>1
(XL(2)≠0 or XH(2)≠0) and (XL(1)<1 and XH(1)≥1
or XL(1)≤1 and XH(1)>1)
XB(3)≤0
ISCLBD≠0 and (XL(3)>XB(3) or XL(3)>XH(3) or XB(3)>XH(3))
ISCLBD<0 and XL(3)≠XH(3)
LOCBND≠0 and (XL(4)>XB(4) or XL(4)>XH(4) or XB(4)>XH(4))
LOCBND<0 and XL(4)≠XH(4)
LOCBND≠0 and XL(1)=XH(1)=1 and (XL(2)≠0 or XH(2)≠0).

On input errors, STABLE terminates immediately, without performing any computations. The second type of error occurs after some computation. IFAULT will be

10 if A was found numerically non positive definite;

11 if A was found ill-conditioned;

12 if too many function evaluations were required during solution of a subproblem;

13 if iteration converged, but the most recent E04KBF fault indicator was 3 and internal checks were not met. These checks are (i) $\|G\|^2$ < 10 * X02AAF(DUMMY), and (ii) K < $1/\|G\|$, as recommended by E04KBF documentation, where $\|G\|$ is the norm of the projected gradient and K the estimated condition number of the projected Hessian matrix;

14 if there were repeated problems with overflow in the Cholesky factors of the projected Hessian;

15 if iteration converged, but the most recent E04KBF fault indicator was 5 and internal checks were not met;

16 if convergence did not occur in MAXIT iterations;

17 if convergence did not occur in MAXIT iterations, the most recent E04KBF fault indicator was 3, and internal checks were not met;

18 if convergence did not occur in MAXIT iterations, the most recent E04KBF fault indicator was 5, and internal checks were not met.

Conditions IFAULT=10 and 11 are detected in SETECF (they are caused by $\tau$ being too small under Formulation B), the remainder in STABLE.

IWORK(2) and IWORK(3) (see Restrictions) are failure indicators for asymptotic covariance matrix versions (i) and (ii) respectively. Zero indicates success, 1 that $\underset{\sim}{H}$ was non positive definite, and 2 that $\underset{\sim}{H}$ was ill-conditioned, the failures detected in SETVCV. If IFAULT=1-12 or 14, covariance matrices are not computed, and their fault indicators are set to the corresponding value of IFAULT.

Auxiliary algorithms

The user has only to call STABLE. Auxiliary procedures fall into two groups: those supplied here, and NAG Library procedures. The following subroutines are supplied:

SUBROUTINE GRIDWT(PAR,NPAR,XLAM,TAU,PTS,NPTS2,WT,NPTS,MODE,KSUM): computes gridpoints and weights;

SUBROUTINE CHARFN(U,PAR,NPAR,RE,XIM): computes real and imaginary parts of standard stable characteristic function $\bar{\phi}(u)$;

SUBROUTINE FUNCT(IFLAG,N,XC,FC,GC,IW,LIW,W,LW): objective function/gradient evaluation;

SUBROUTINE SETECF(X,N,PAR,NPAR,MODE,TAU,SIGMA,XMU,KSUM,IA,NPTS2,NPTS, PTS,ECF,A,AINV,WORK,IFAULT): computes standardized empirical characteristic function values $\tilde{\psi}_n^k(u)$, computes and inverts A under Formulation B;

SUBROUTINE MONIT(N,XC,FC,GC,ISTATE,GPJNRM,COND,POSDEF,NITER,NF,IW,LIW, W,LW): monitors the progress of E04KBF;

SUBROUTINE VARIAB(ICOV,X,N,PAR,NPAR,MODE,SIGMA,XMU,ISUB,NVAR,PTS,NPTS2, WT,ECF,NPTS,DERIV,WORK,HOLD,A,IA,AINV,VCV1,VCV2,H,NVAR1,V,IW,LIW,W,LW, IFAIL1,IFAIL2): computes approximate asymptotic covariance matrices;

SUBROUTINE VMATRX (X,N,MODE,XMU,SIGMA,PTS,NPTS2,WT,ECF,WORK,NPTS,DERIV, V,HOLD,NVAR): computes $\tilde{V}$ for version (i) of asymptotic covariance matrix;

SUBROUTINE DAPROD(FAC1,IFAC1,NPTS,FAC2,WORK,NVAR): auxiliary matrix multiplication for VARIAB:

SUBROUTINE HVPROD(FAC1,IFAC1,NVAR,FAC2,NPTS,VH,IVH): auxiliary matrix multiplication for VARIAB;

SUBROUTINE SETVCV(ISUB,NVAR,H,NVAR1,V,WORK,VCV,NPAR,SIGMA,IFAULT): auxiliary routine for VARIAB;

SUBROUTINE HESDIF(PAR,NPAR,ISUB,H,SAVE1,SAVE2,NVAR,IW,LIW,W,LW): computes an approximate Hessian by differencing for version (i) of asymptotic covariance matrix.

The following NAG Library procedures are used:

REAL FUNCTION X02AAF(DUMMY): returns the smallest positive $\epsilon$ such that $1.0 + \epsilon > 1.0$;

SUBROUTINE E04KBF(N,FUNCT,MONIT,IPRINT,LOCSCH,INTYPE,MINLIN,MAXCAL,ETA, XTOL,STEPMX,FEST,IBOUND,BL,BU,X,HESL,LH,HESD,ISTATE,F,G,IW,LIW,W,LW,IFAIL): solves optimization problems. Control parameters are set as follows:

| | | |
|---|---|---|
| IPRINT | = | 0 |
| LOCSCH | = | .TRUE. |
| INTYPE | = | 3 for subproblems after the first if parameters which are not fixed are not on bounds, else 0 |
| MINLIN | = | NAG Library routine E04LBS |
| MAXCAL | = | 400 |
| ETA | = | 0.9 |
| XTOL | = | $10.0\sqrt{\text{X02AAF(DUMMY)}}$ explicitly, so it is available on exit |
| STEPMX | = | 0.25 |
| FEST | = | 0.0 |
| IBOUND | = | 0 ; |

SUBROUTINE F01ABF(A,IA,N,B,IB,Z,IFAIL): inverts the positive definite symmetric matrix A;

SUBROUTINE F01CAF(A,M,N,IFAIL): sets matrix A to zero;

SUBROUTINE F01CMF(A,LA,B,LB,M,N): copies elements of matrix A into matrix B;

SUBROUTINE F01CKF(A,B,C,N,IP,M,Z,IZ,IOPT,IFAIL): matrix multiplication A=BC, where B or C may be overwritten.

## RESTRICTIONS

We require the sample size N at least 50, since for smaller samples $\tilde{\psi}_n(u)$ is not generally sufficiently smooth to allow accurate estimation. Since $\tilde{\alpha}$ and $\tilde{\beta}$ are bounded in the narrow ranges (0,2] and [-1,1] and have standard errors decreasing as $N^{-\frac{1}{2}}$, it is preferable to have N≥100. For N less than 150, say, relatively large values of $\lambda$ may be preferred, to damp out noise in $\tilde{\psi}_n(u)$. We further require NPTS≥20.

Extended work vectors WORK and IWORK are required, in order to communicate information to FUNCT and MONIT without using COMMON blocks. To aid readers who may wish to adapt the algorithm to installations not having the NAG Library, we describe the use of these work vectors.

The required length of WORK is 10 + 11*NPAR + NPAR*(NPAR-1)/2 + (3+NPAR)*NPTS + NPTS + NPTS/2 if MODE≠0, with an additional NPTS*(2*NPTS+1) required if MODE=0. Some sample lengths are

| MODE | NPTS=20 | NPTS=40 |
|---|---|---|
| 0 | 1030 | 3600 |
| nonzero | 210 | 360 |

The subvector W is passed to E04KBF,FUNCT, and MONIT.

| WORK starting point | W starting point | Elements | Used for |
|---|---|---|---|
| 1 | - | 1 | Convergence criterion |
| 2 | - | 1 | Objective function value on exit from E04KBF |
| 3 | - | NPAR | Projected gradient on exit from E04KBF |
| (other addresses internally computed) | - | 1 | Old $\tilde{\alpha}$ value for convergence testing |
| | - | 1 | Old $\tilde{\beta}$ value for convergence testing |
| | - | 1 | $\tilde{\sigma}$ lower bound on entry |
| | - | 1 | $\tilde{\sigma}$ upper bound on entry |
| | - | 1 | $\tilde{\mu}$ lower bound on entry |
| | - | 1 | $\tilde{\mu}$ upper bound on entry |
| | - | NPAR*(NPAR-1)/2 | HESL factor for E04KBF |
| | - | NPAR | HESD factor for E04KBF; workspace for VARIAB |
| | 1 (other addresses internally computed) | 9*NPAR | E04KBF workspace; broken up into H and V matrices and used as workspace in VARIAB |
| | | 1 | On exit from E04KBF, estimated condition number of projected Hessian |
| | | 1 | On exit from E04KBF, norm of projected gradient |
| | | NPTS/2 | Positive gridpoints PTS |
| | | NPTS | Weights WT |
| | | NPTS | Empirical characteristic function values ECF, workspace in VARIAB |
| | | NPAR*NPTS | Partial derivatives of $\psi(u)$ at gridpoints, workspace in VARIAB |
| | | NPTS | Workspace for FUNCT and VARIAB |
| | | (NPTS+1)*NPTS | If MODE=0, used for A matrix (the extra row is required by NAG Library routine F01ABF); workspace in VARIAB |
| | | NPTS*NPTS | If MODE=0, used for $A^{-1}$; workspace in VARIAB |

The required length of IWORK is 7 + NPAR. The subvector IW is passed to E04KBF, FUNCT, and MONIT.

| IWORK starting point | IW starting point | Elements | Use for |
|---|---|---|---|
| 1 | - | 1 | Iteration count |
| 2 | - | NPAR | ISTATE vector for E04KBF, workspace for VARIAB. If covariance matrices are requested, on exit IWORK(2) contains a fault indicator for approximation (i), IWORK(3) contains a fault indicator for approximation (ii), and IWORK(4) contains the number of iterations required to compute the approximate Hessian for approximation (i) |
| (other addresses internally computed) | | | |
| | 1 | 2 | Workspace for E04KBF, HESDIF |
| | 3 | 1 | Stores MODE |
| | 4 | 1 | Stores output unit number IUNIT |
| | 5 | 1 | Stores NPTS |
| | 6 | 1 | Stores 1 less than the address of PTS(1) in W |

## PRECISION

Double precision will be required on computers with 32 bit wordlength. The precision used by the local NAG Library implementation should be adequate. To change the precision:

- change all REAL declarations to DOUBLE PRECISION;
- replace constants by double precision versions, constants $\frac{\pi}{2}$, $\frac{2}{\pi}$, $\sqrt{10}$ typed in to machine accuracy;
- declare NAG Library function X02AAF as DOUBLE PRECISION;
- change the precision of FORTRAN library functions, i.e., ABS to DABS, ATAN2 to DATAN2, SIGN to DSIGN, etc. FLOAT(I) can be replaced by DBLE(FLOAT(I)).

If extremely large observations are present in the sample, there may be a loss of significant figures when computing sines and cosines in SETECF and VMATRX. This should not occur when real data is used, but can be a problem with simulated data for small $\alpha$.

## TIME

Execution times depend on the quality of initial guesses and properties of the real data used, and vary somewhat throughout the parameter space. As a rough guide, we give some statistics for simulated data, using a moderately difficult situation with $\alpha>1$. Tables 1a and 1b provide approximate running times for Formulation A, q=40, and Formulation B, q=20, n=100,200,500,1000,2500. Timing starts upon entry to STABLE. Samples from S(1.3,-.5,3,15) were generated using the method of Chambers, Mallows, and Stuck (1976). Initial guesses for $\alpha,\beta,\sigma,\mu$ in all cases were 1.505=½(1.01+2), 0, $\frac{1}{2}(x_{.75}-x_{.25})$, and $x_{.5}$, the sample median, respectively. Because of skewness, the median is not a good estimator of $\mu$ in this case. Five iterations were used. Time required to compute asymptotic covariance matrices includes approximations (i) and (ii), except where noted. Timings are for a double precision version of the algorithm, compiled by the IBM FORTRAN H Extended compiler, and run on an IBM 370/3033.

The following qualitative points are clear from this rather restricted set of timings. There is a substantial overhead, which may crudely be assumed fixed, associated with nonlinear optimization, although E04KBF solves the optimization subproblems rapidly. For large samples, run time is dominated by evaluation of the empirical characteristic function, and thus is asymptotically linear in n for a fixed number of iterations.

Table 1a

Timings for Formulation A, q=40, on Simulated Samples from s(1.3,-.5,3,15); $\lambda$=1 for n≤200 and .5 for n>200, $\tau$=1

| n | Iterations | Estimation time (sec) | Convergence criterion | Covariance matrix time |
|---|---|---|---|---|
| 100 | 5 | 0.7 | 5.4(-4) | 0.1* |
| 200 | 5 | 1.0 | 2.3(-2) | 0.1* |
| 500 | 5 | 1.8 | 1.8(-4) | 0.8 |
| 1000 | 5 | 3.2 | 3.3(-5) | 1.2 |
| 2500 | 5 | 7.5 | 4.8(-6) | 2.5 |

*Sample size too small to compute approximation (i), only approximation (ii) computed.

Table 1b

Timings for Formulation B, q=20, on Simulated Samples from s(1.3,-.5,3,15); $\lambda=\tau=0$

| n | Iterations | Estimation time (sec) | Convergence criterion | Covariance matrix time |
|---|---|---|---|---|
| 100 | 5 | 0.9 | 1.2(-2) | 0.3 |
| 200 | 5 | 1.2 | 3.2(-2) | 0.4 |
| 500 | 5 | 1.6 | 1.8(-4) | 0.5 |
| 1000 | 5 | 2.3 | 5.7(-5) | 0.7 |
| 2500 | 5 | 4.4 | 1.5(-4) | 1.4 |

Approximation (ii) of the asymptotic covariance matrix is quite easy to compute, while approximation (i) is highly time-consuming.

For fixed k>1 with the k-sum procedure, one iteration generally suffices, provided estimates from the nearest value of k are used, and the estimates don't change much. For mixtures of very different distributions, or if the exponent $\tilde{\alpha}$ is near unity, more are required.

## ADDITIONAL COMMENTS

Although output need not be produced, we recommend calling STABLE with IUNIT>0, so the user will have a record of how estimation progressed. The following information will then be printed out:

by MONIT: number of E04KBF iterations and function evaluations, objective function value, norm of projected gradient, subproblem solution, projected gradient, and estimated condition number of projected Hessian;

by STABLE: E04KBF fault indicator, and value of convergence criterion;

by HESDIF(if called): number of iterations needed to compute approximate Hessian, and steplength used.

Use of STABLE in "batch mode" has drawbacks. For instance, most faults arising in E04KBF are not diagnosed until iteration ceases. In practice, such faults may likely be due to the initial $\tilde{\alpha}$ being on the wrong side of 1. Further, when $\tilde{\alpha}$ is small, convergence tolerances are difficult to interpret, and the user may prefer direct control of iteration. We therefore prefer to use STABLE interactively, a copy of the output described above being directed to the terminal, and the user deciding after each iteration whether he wishes to continue. Required modifications are simple.

Faster and/or more compact codings of the Algorithm are possible, for instance, if $\beta$ is known to be zero, if only Formulation A or Formulation B is desired, or if asymptotic covariance matrices are not desired. Generality is achieved at a price in efficiency.

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C*************************************************************************STAB 001
C        CENTRAL SUBROUTINE OF ESTIMATION PROCESS.                        STAB 002
C        CALLED BY - MAIN                                                 STAB 003
C        CALLS - GRIDWT, SETECF, VARIAB                                   STAB 004
C        PASSES TO E04KBF VIA EXTERNAL STMT - FUNCT, MONIT, E04LBS        STAB 005
C        N.A.G. PROCEDURES CALLED -                                       STAB 006
C               X02AAF (RETURNS MACHINE PRECISION),                       STAB 007
C               E04KBF (QUASI-NEWTON OPTIMIZATION WITH BOUNDED            STAB 008
C                       VARIABLES),                                       STAB 009
C               F01CAF (SETS A MATRIX TO ZERO).                           STAB 010
C*************************************************************************STAB 011
      SUBROUTINE STABLE(X, N, MODE, KSUM, XLAM, TAU, NPTS, TOL, MAXIT,    STAB 012
     *XL, XB, XH, NPAR, ISCLBD, LOCBND, ICOV, VCV1, VCV2, WORK, LWORK,    STAB 013
     *IWORK, LIWORK, IUNIT, IFAULT)                                       STAB 014
C        EXTERNAL ROUTINES                                                STAB 015
      EXTERNAL E04LBS, FUNCT, MONIT                                       STAB 016
C        ARGUMENTS                                                        STAB 017
      INTEGER N, MODE, KSUM, NPTS, MAXIT, NPAR, ISCLBD, LOCBND, ICOV,     STAB 018
     *LWORK, LIWORK, IWORK(LIWORK), IUNIT, IFAULT                         STAB 019
      REAL X(N), XLAM, TAU, TOL, XL(NPAR), XB(NPAR), XH(NPAR),            STAB 020
     *VCV1(NPAR,NPAR), VCV2(NPAR,NPAR), WORK(LWORK)                       STAB 021
C        FUNCTION CALLED                                                  STAB 022
      REAL X02AAF                                                         STAB 023
C        LOCAL SCALARS                                                    STAB 024
C        SPECIFICALLY FOR E04KBF PARAMETERS -                             STAB 025
      LOGICAL LOCSCH                                                      STAB 026
      INTEGER LW, LIW, MAXCAL, IBOUND, IPRINT, LHESL, INTYPE              STAB 027
      REAL ETA, XTOL, STEPMX, FEST                                        STAB 028
C        SCRATCH VARIABLES, SUBSCRIPT INDICATORS, AND CONSTANTS -         STAB 029
      INTEGER IND, IND1, IOVFLW, NPTS2, IA, NVAR, NVAR1, MPTS, MWT,       STAB 030
     *MECF, MDERIV, MVWORK, MA, MAINV, MHESL, MHESD, MIW, MW, MV          STAB 031
      REAL SIGMA, XMU, XK, ZERO, PT2, TWOVPI, ONE, TWO, SQRT10, FIVE,     STAB 032
     *TEN                                                                 STAB 033
      DATA LOCSCH, MAXCAL, IBOUND, IPRINT, ETA, STEPMX, FEST              STAB 034
     */.TRUE., 400, 0, 0, 0.9, 0.25, 0.0/                                 STAB 035
      DATA ZERO, PT2, TWOVPI, ONE, TWO, SQRT10, FIVE, TEN                 STAB 036
     */0.0, 0.2, 0.6366197724, 1.0, 2.0, 3.162277660, 5.0, 10.0/          STAB 037
C                                                                         STAB 038
C        ON INPUT ERRORS (IFAULT = 1 - 9), EXIT IMMEDIATELY.              STAB 039
      IWORK(1) = 0                                                        STAB 040
      WORK(1) = ZERO                                                      STAB 041
      IFAULT = 1                                                          STAB 042
      IF (MAXIT .LE. 0) RETURN                                            STAB 043
      IFAULT = 2                                                          STAB 044
      IF (N .LT. 50) RETURN                                               STAB 045
      IFAULT = 3                                                          STAB 046
      IF (KSUM .LE. 0) RETURN                                             STAB 047
      IFAULT = 4                                                          STAB 048
      IF (TAU .LT. ZERO .OR. MODE .NE. 0 .AND. TAU .GT. ONE) RETURN       STAB 049
      IFAULT = 5                                                          STAB 050
      IF (NPTS .LT. 20 .OR. MOD(NPTS,2) .NE. 0) RETURN                    STAB 051
      IFAULT = 6                                                          STAB 052
      IF (TOL .LE. ZERO) RETURN                                           STAB 053
      IFAULT = 7                                                          STAB 054
      IF (NPAR .NE. 4) RETURN                                             STAB 055
      IFAULT = 8                                                          STAB 056
      NPTS2 = NPTS / 2                                                    STAB 057
      LHESL = (NPAR*NPAR - NPAR) / 2                                      STAB 058
      LW = 10 + 11 * NPAR + LHESL + (3 + NPAR) * NPTS + NPTS2             STAB 059
      IF (MODE .EQ. 0) LW = LW + NPTS * (2*NPTS + 1)                      STAB 060
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```
      IF (LWORK .LT. LW .OR. LIWORK .LT. NPAR + 7) RETURN                STAB 061
C                                                                        STAB 062
C        CHECKING OF PARAMETER BOUNDS (IFAULT = 9 IF WRONG)              STAB 063
      IFAULT = 9                                                         STAB 064
      IF (XL(1) .GT. XB(1) .OR. XL(1) .GT. XH(1) .OR. XB(1) .GT. XH(1)) STAB 065
     *RETURN                                                             STAB 066
      IF (XL(1) .LE. ZERO .OR. XH(1) .GT. TWO) RETURN                    STAB 067
      IF (XL(2) .GT. XB(2) .OR. XL(2) .GT. XH(2) .OR. XB(2) .GT. XH(2)) STAB 068
     *RETURN                                                             STAB 069
      IF (XL(2) .LT. - ONE .OR. XH(2) .GT. ONE) RETURN                   STAB 070
      IF ((XL(2) .NE. ZERO .OR. XH(2) .NE. ZERO) .AND. (XL(1) .LT. ONE   STAB 071
     *.AND. XH(1) .GE. ONE .OR. XL(1) .LE. ONE .AND. XH(1) .GT. ONE))    STAB 072
     *RETURN                                                             STAB 073
      IF (XB(3) .LE. ZERO) RETURN                                        STAB 074
      IF (ISCLBD .NE. 0 .AND. (XL(3) .GT. XB(3) .OR. XL(3) .GT. XH(3) .  STAB 075
     *OR. XB(3) .GT. XH(3))) RETURN                                      STAB 076
      IF (ISCLBD .LT. 0 .AND. XL(3) .NE. XH(3)) RETURN                   STAB 077
      IF (LOCBND .NE. 0 .AND. (XL(4) .GT. XB(4) .OR. XL(4) .GT. XH(4) .  STAB 078
     *OR. XB(4) .GT. XH(4))) RETURN                                      STAB 079
      IF (LOCBND .LT. 0 .AND. XL(4) .NE. XH(4)) RETURN                   STAB 080
      IF (LOCBND .NE. 0 .AND. XL(1) .EQ. ONE .AND. XH(1) .EQ. ONE .AND.  STAB 081
     *(XL(2) .NE. ZERO .OR. XL(2) .NE. XH(2))) RETURN                    STAB 082
C                                                                        STAB 083
C        INITIAL ADJUSTMENT OF LOCATION/SCALE PARAMETERS/BOUNDS.         STAB 084
C        SAVE BOUNDS FOR EXIT.                                           STAB 085
      WORK(NPAR + 5) = XL(3)                                             STAB 086
      WORK(NPAR + 6) = XH(3)                                             STAB 087
      WORK(NPAR + 7) = XL(4)                                             STAB 088
      WORK(NPAR + 8) = XH(4)                                             STAB 089
      XK = FLOAT(KSUM)                                                   STAB 090
C        LOCATION                                                        STAB 091
      XMU = XK * XB(4)                                                   STAB 092
      IF (LOCBND .LT. 0) GO TO 10                                        STAB 093
      IF (LOCBND .GT. 0) GO TO 20                                        STAB 094
      XL(4) = -FIVE                                                      STAB 095
      XH(4) = FIVE                                                       STAB 096
      GO TO 30                                                           STAB 097
   10 XL(4) = ZERO                                                       STAB 098
      XH(4) = ZERO                                                       STAB 099
      GO TO 30                                                           STAB 100
   20 XL(4) = XK * XL(4)                                                 STAB 101
      XH(4) = XK * XH(4)                                                 STAB 102
C        SCALE                                                           STAB 103
   30 XTOL = XK ** (ONE/XB(1))                                           STAB 104
      SIGMA = XTOL * XB(3)                                               STAB 105
      IF (ISCLBD .LT. 0) GO TO 40                                        STAB 106
      IF (ISCLBD .GT. 0) GO TO 50                                        STAB 107
      XL(3) = PT2                                                        STAB 108
      XH(3) = FIVE                                                       STAB 109
      GO TO 60                                                           STAB 110
   40 XL(3) = ONE                                                        STAB 111
      XH(3) = ONE                                                        STAB 112
      GO TO 60                                                           STAB 113
   50 XL(3) = XTOL * XL(3)                                               STAB 114
      XH(3) = XTOL * XH(3)                                               STAB 115
C                                                                        STAB 116
C        EXPLICITLY SET XTOL TO E04KBF DEFAULT VALUE, USING X02AAF,      STAB 117
C        SO THAT IT IS AVAILABLE ON EXIT ON E04KBF.                      STAB 118
   60 XTOL = TEN * SQRT(X02AAF(XTOL))                                    STAB 119
C                                                                        STAB 120
```

```
C        MEMORY MANAGEMENT                                                  STAB 121
      MIW = 2 + NPAR                                                        STAB 122
      IWORK(MIW + 2) = MODE                                                 STAB 123
      IWORK(MIW + 3) = IUNIT                                                STAB 124
      IWORK(MIW + 4) = NPTS                                                 STAB 125
      IWORK(MIW + 5) = 9 * NPAR + 2                                         STAB 126
      LIW = 6                                                               STAB 127
      LW = LW - 8 - 2 * NPAR - LHESL                                        STAB 128
      MHESL = 9 + NPAR                                                      STAB 129
      MHESD = MHESL + LHESL                                                 STAB 130
      MW = MHESD + NPAR                                                     STAB 131
      MPTS = MW + 9 * NPAR + 2                                              STAB 132
      MWT = MPTS + NPTS2                                                    STAB 133
      MECF = MWT + NPTS                                                     STAB 134
      MDERIV = MECF + NPTS                                                  STAB 135
C        AVOID UNCLEAR REFERENCES TO A AND A INVERSE IF MODE .NE. 0         STAB 136
      MA = MDERIV                                                           STAB 137
      MAINV = MDERIV                                                        STAB 138
      IA = NPTS + 1                                                         STAB 139
      IF (MODE .NE. 0) GO TO 70                                             STAB 140
      MA = MA + (NPAR + 1) * NPTS                                           STAB 141
      MAINV = MA + IA * NPTS                                                STAB 142
C        LOOPING POINT FOR ITERATION                                        STAB 143
   70 IWORK(1) = IWORK(1) + 1                                               STAB 144
      IOVFLW = 0                                                            STAB 145
C                                                                           STAB 146
C        IF LOCATION/SCALE PARAMETERS ARE CONSTRAINED, UPDATE               STAB 147
C        THEIR BOUNDS.                                                      STAB 148
      IF (ISCLBD .LE. 0) GO TO 80                                           STAB 149
      XL(3) = AMIN1(ONE,AMAX1(PT2,WORK(NPAR + 5)/SIGMA))                    STAB 150
      XH(3) = AMAX1(ONE,AMIN1(FIVE,WORK(NPAR + 6)/SIGMA))                   STAB 151
   80 IF (LOCBND .LE. 0) GO TO 90                                           STAB 152
      XL(4) = AMIN1(ZERO,AMAX1(-FIVE,(WORK(NPAR + 7) - XMU)/SIGMA))         STAB 153
      XH(4) = AMAX1(ZERO,AMIN1(FIVE,(WORK(NPAR + 8) - XMU)/SIGMA))          STAB 154
C        CHANGE PARAMETERS TO REFLECT FUTURE STANDARDIZATION.               STAB 155
   90 XB(3) = ONE                                                           STAB 156
      XB(4) = ZERO                                                          STAB 157
      WORK(NPAR + 3) = XB(1)                                                STAB 158
      WORK(NPAR + 4) = XB(2)                                                STAB 159
C        SET INTYPE = 3 IF POSSIBLE, SO OLD HESSIAN CAN BE USED.            STAB 160
      INTYPE = 0                                                            STAB 161
      IF (IWORK(1) .EQ. 1) GO TO 110                                        STAB 162
      INTYPE = 3                                                            STAB 163
      DO 100 I = 1, NPAR                                                    STAB 164
      IF (IWORK(I + 1) .GT. 0) GO TO 100                                    STAB 165
      INTYPE = 0                                                            STAB 166
      GO TO 110                                                             STAB 167
  100 CONTINUE                                                              STAB 168
C                                                                           STAB 169
C        SET GRIDPOINTS, WEIGHTS.                                           STAB 170
  110 CALL GRIDWT(XB, NPAR, XLAM, TAU, WORK(MPTS), NPTS2, WORK(MWT),        STAB 171
     *NPTS, MODE, KSUM)                                                     STAB 172
C        SET E. CH. F. VALUES, ALSO A AND A INVERSE, IF MODE = 0, USING     STAB 173
C        FIRST COL. OF DERIV AS WORKSPACE.                                  STAB 174
      CALL SETECF(X, N, XB, NPAR, MODE, TAU, SIGMA, XMU, KSUM, IA,          STAB 175
     *NPTS2, NPTS, WORK(MPTS), WORK(MECF), WORK(MA), WORK(MAINV),           STAB 176
     *WORK(MDERIV), IFAULT)                                                 STAB 177
      IF (IFAULT .GT. 0) IFAULT = 9 + IFAULT                                STAB 178
      IF (IFAULT .EQ. 10 .OR. IFAULT .EQ. 11) GO TO 180                     STAB 179
C                                                                           STAB 180
```

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C        CALL OR RESTART N.A.G. ROUTINE E04KBF                                  STAB 181
  120 IFAULT = 1                                                                 STAB 182
      CALL E04KBF(NPAR, FUNCT, MONIT, IPRINT, LOCSCH, INTYPE, E04LBS,            STAB 183
     *MAXCAL, ETA, XTOL, STEPMX, FEST, IBOUND, XL, XH, XB, WORK(MHESL),          STAB 184
     *LHESL, WORK(MHESD), IWORK(2), WORK(2), WORK(3), IWORK(MIW), LIW,           STAB 185
     *WORK(MW), LW, IFAULT)                                                      STAB 186
C        COMPUTE CONVERGENCE CRITERION                                          STAB 187
      WORK(1) = AMAX1(ABS(XB(3) - ONE),ABS(XB(4)))                              STAB 188
      IF (ISCLBD .LT. 0 .AND. LOCBND .LT. 0) WORK(1) = AMAX1(ABS(XB(1) -STAB 189
     * WORK(NPAR + 3)),ABS(XB(2) - WORK(NPAR + 4)))                             STAB 190
C        OUTPUT IF REQUESTED                                                    STAB 191
      IF (IUNIT .GT. 0) WRITE (IUNIT,1000) IWORK(1), IFAULT, WORK(1)            STAB 192
      IF (IFAULT .EQ. 0) GO TO 140                                              STAB 193
C        IF E04KBF FAULT INDICATOR IS 2, 3, 4, OR 5, JUDGE QUALITY              STAB 194
C        OF SOLUTION.  NOTE IFAULT = 1 IS IMPOSSIBLE.                           STAB 195
      IFAULT = 10 + IFAULT                                                      STAB 196
C        IF MAXCAL FUNCTION EVALUATIONS HAVE BEEN MADE, GIVE UP                 STAB 197
      IF (IFAULT .EQ. 12) GO TO 180                                             STAB 198
      IF (IFAULT .NE. 14) GO TO 130                                             STAB 199
C        ONE OVERFLOW IN HESSIAN CHOLESKY FACTORS IS ALLOWED                    STAB 200
      IF (IOVFLW .GE. 1) GO TO 180                                              STAB 201
      IOVFLW = IOVFLW + 1                                                       STAB 202
      INTYPE = 0                                                                STAB 203
      GO TO 120                                                                 STAB 204
C        IF IFAULT = 13 OR 15, TEST PROJECTED GRADIENT AND PROJECTED            STAB 205
C        HESSIAN CONDITION NUMBER                                               STAB 206
  130 IND = MW + 9 * NPAR                                                       STAB 207
      IF (SQRT10*WORK(IND + 1) .LT. XTOL .AND. WORK(IND) .LT. ONE/WORK( STAB 208
     *IND + 1)) IFAULT = 0                                                      STAB 209
C                                                                               STAB 210
C        UPDATE LOCATION AND SCALE AND TEST CONVERGENCE                         STAB 211
  140 XMU = XMU + SIGMA * XB(4)                                                 STAB 212
      IF (XB(1) .EQ. ONE) XMU = XMU + SIGMA * TWOVPI * XB(2) * XB(3) *  STAB 213
     *ALOG(XB(3))                                                               STAB 214
      SIGMA = SIGMA * XB(3)                                                     STAB 215
      IF (WORK(1) .LT. TOL) GO TO 150                                           STAB 216
      IF (IWORK(1) .LT. MAXIT) GO TO 70                                         STAB 217
C                                                                               STAB 218
C        MAXIT ITNS HAVE BEEN USED WITHOUT CONVERGENCE - SET IFAULT.            STAB 219
      IND = 16                                                                  STAB 220
      IF (IFAULT .EQ. 13) IND = 17                                              STAB 221
      IF (IFAULT .EQ. 15) IND = 18                                              STAB 222
      IFAULT = IND                                                              STAB 223
C                                                                               STAB 224
C        TERMINATION WITH IFAULT = 0, 13, 15, 16, 17 OR 18                      STAB 225
  150 IF (KSUM .GT. 1 .OR. ICOV .LT. 0) GO TO 190                               STAB 226
C                                                                               STAB 227
C        PREPARE TO CALL VARIAB TO COMPUTE COVARIANCE MATRICES.                 STAB 228
C        MEMORY MANAGEMENT.                                                     STAB 229
      MVWORK = MDERIV + NPAR * NPTS                                             STAB 230
      MV = MW + NPAR * (NPAR + 1)                                               STAB 231
C                                                                               STAB 232
C        REARRANGE THE N.A.G. ISTATE VECTOR SO IT HOLDS FREE                    STAB 233
C        PARAMETER SUBSCRIPTS IN INCREASING ORDER.                              STAB 234
      NVAR = 0                                                                  STAB 235
      DO 160 I = 1, NPAR                                                        STAB 236
      IF (IWORK(I + 1) .LT. 0) GO TO 160                                        STAB 237
      NVAR = NVAR + 1                                                           STAB 238
      IWORK(NVAR + 1) = I                                                       STAB 239
  160 CONTINUE                                                                  STAB 240
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C        IN THE RARE EVENT THAT THERE ARE NO FREE VARIABLES, VARIAB      STAB 241
C        IS NOT CALLED AND COVARIANCE MATRICES ARE SET TO ZERO.          STAB 242
      IF (NVAR .GT. 0) GO TO 170                                         STAB 243
      IF (ICOV .EQ. 0) CALL F01CAF(VCV1, NPAR, NPAR, IWORK(2))           STAB 244
      CALL F01CAF(VCV2, NPAR, NPAR, IWORK(3))                            STAB 245
      GO TO 190                                                          STAB 246
  170 NVAR1 = NVAR + 1                                                   STAB 247
      XB(3) = ONE                                                        STAB 248
      XB(4) = ZERO                                                       STAB 249
C                                                                        STAB 250
C        COMPUTE ESTIMATED ASYMPTOTIC COVARIANCE MATRICES.               STAB 251
      CALL VARIAB(ICOV, X, N, XB, NPAR, MODE, SIGMA, XMU, IWORK(2),      STAB 252
     *NVAR, WORK(MPTS), NPTS2, WORK(MWT), WORK(MECF), NPTS,              STAB 253
     *WORK(MDERIV), WORK(MVWORK), WORK(MHESD), WORK(MA), IA,             STAB 254
     *WORK(MAINV), VCV1, VCV2, WORK(MW), NVAR1, WORK(MV), IWORK(MIW),    STAB 255
     *LIW, WORK(MW), LW, IND, IND1)                                      STAB 256
C        SAVE FAULT INDICATORS AND NO. OF ITNS TAKEN FOR HESSIAN.        STAB 257
      IWORK(2) = IND                                                     STAB 258
      IWORK(3) = IND1                                                    STAB 259
      IWORK(4) = IWORK(MIW)                                              STAB 260
      GO TO 190                                                          STAB 261
C                                                                        STAB 262
C        EXIT FOR IFAULT = 10, 11, 12, OR 14.  IF IFAULT = 12 OR 14,     STAB 263
C        RESULTS OF THE LAST (ABORTED) OPTIMIZATION ARE NOT USED.        STAB 264
  180 IWORK(2) = IFAULT                                                  STAB 265
      IWORK(3) = IFAULT                                                  STAB 266
C                                                                        STAB 267
C        EXIT FOR IFAULT = 0, 13, 15, 16, 17, OR 18.                     STAB 268
C        RESET LOCATION/SCALE BOUNDS                                     STAB 269
  190 XL(3) = WORK(NPAR + 5)                                             STAB 270
      XH(3) = WORK(NPAR + 6)                                             STAB 271
      XL(4) = WORK(NPAR + 7)                                             STAB 272
      XH(4) = WORK(NPAR + 8)                                             STAB 273
C        ADJUST PARAMETERS TO STANDARD FORM                              STAB 274
      IF (XB(1) .EQ. ONE) XMU = XMU - TWOVPI * XB(2) * SIGMA * ALOG(     STAB 275
     *SIGMA)                                                             STAB 276
      XB(4) = XMU / XK                                                   STAB 277
      XB(3) = SIGMA / (XK**(ONE/XB(1)))                                  STAB 278
C                                                                        STAB 279
 1000 FORMAT (10HOMAJOR ITN, I3, 18H, IFAIL (E04KBF) =, I3,              STAB 280
     *25H, CONVERGENCE CRITERION =, E11.3)                               STAB 281
      RETURN                                                             STAB 282
      END                                                                STAB 283
C*********************************************************************GRID 001
C        CALCULATES (POSITIVE) GRIDPOINTS AND ALL WEIGHTS.               GRID 002
C        CALLED BY - STABLE                                              GRID 003
C        CALLS - CHAREN                                                  GRID 004
C*********************************************************************GRID 005
      SUBROUTINE GRIDWT(PAR, NPAR, XLAM, TAU, PTS, NPTS2, WT, NPTS,      GRID 006
     *MODE, KSUM)                                                        GRID 007
C        ARGUMENTS                                                       GRID 008
      INTEGER NPAR, NPTS2, NPTS, MODE, KSUM                              GRID 009
      REAL PAR(NPAR), XLAM, TAU, PTS(NPTS2), WT(NPTS)                    GRID 010
C        LOCAL SCALARS                                                   GRID 011
      LOGICAL FLAG                                                       GRID 012
      INTEGER IND, IND1, IND2, INNER                                     GRID 013
      REAL ALPHA, AFAC1, AFAC2, TEMP, GAP, END, C1                       GRID 014
C        CONSTANTS                                                       GRID 015
      REAL ZERO, PT025, PT035, PT04, PT0425, PT045, PT05, PT06, PT07,    GRID 016
     *PT075, PT3, PT5, PT6, PT8, PT9, ONE, ONEPT2, ONEPT4, ONEPT6,      GRID 017
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     *ONEPT7, ONEPT8, TWO, THREE, THRPT3, THRPT6, FOUR, FIVE, SEVEN, TENGRID 018
      DATA ZERO, PT025, PT035, PT04, PT0425, PT045, PT05, PT06, PT07,   GRID 019
     *PT075, PT3, PT5, PT6, PT8, PT9, ONE, ONEPT2, ONEPT4, ONEPT6,     GRID 020
     *ONEPT7, ONEPT8, TWO, THREE, THRPT3, THRPT6, FOUR, FIVE, SEVEN,   GRID 021
     *TEN /0.0, 0.025, 0.035, 0.04, 0.0425, 0.045, 0.05, 0.06, 0.07,  GRID 022
     *0.075, 0.3, 0.5, 0.6, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6, 1.7, 1.8, 2.0,GRID 023
     *3.0, 3.3, 3.6, 4.0, 5.0, 7.0, 10.0/                             GRID 024
C                                                                     GRID 025
C        SELECT NUMBER OF INNER GRIDPOINTS.                           GRID 026
C        NUMBER OF INNER PTS = 2 IF NPTS .LT. 30, 3 IF NPTS .GE. 30.  GRID 027
      INNER = 2                                                       GRID 028
      IF (NPTS .GE. 30) INNER = 3                                     GRID 029
      ALPHA = PAR(1)                                                  GRID 030
      IF (ALPHA .LE. ONE) GO TO 70                                    GRID 031
C                                                                     GRID 032
C        CASE WHEN ALPHA .GT. 1 - FIRST CHOOSE RIGHT ENDPOINT.        GRID 033
      END = THREE                                                     GRID 034
      IF (ALPHA .LT. ONEPT8) END = THRPT3                             GRID 035
      IF (ALPHA .LT. ONEPT7) END = THRPT6                             GRID 036
      IF (KSUM .EQ. 1) GO TO 20                                       GRID 037
C                                                                     GRID 038
C        WHEN KSUM = 1, EQUISPACE POINTS.                             GRID 039
      TEMP = ZERO                                                     GRID 040
      GAP = END / FLOAT(NPTS2)                                        GRID 041
      DO 10 I = 1, NPTS2                                              GRID 042
      TEMP = TEMP + GAP                                               GRID 043
      PTS(I) = TEMP                                                   GRID 044
   10 CONTINUE                                                        GRID 045
      GO TO 100                                                       GRID 046
C                                                                     GRID 047
C        WHEN KSUM .GT. 1 - FIRST USE HALF OF F-M ALPHA OPTIMAL GAPS  GRID 048
C        FOR POINTS CLOSE TO ORIGIN.                                  GRID 049
   20 IF (NPTS .GE. 30) GO TO 30                                      GRID 050
      GAP = PT075                                                     GRID 051
      IF (ALPHA .LT. ONEPT8) GAP = PT06                               GRID 052
      IF (ALPHA .LT. ONEPT6) GAP = PT07                               GRID 053
      IF (ALPHA .LT. ONEPT4) GAP = PT075                              GRID 054
      IF (ALPHA .LT. ONEPT2) GAP = PT0425                             GRID 055
      GO TO 40                                                        GRID 056
   30 GAP = PT05                                                      GRID 057
      IF (ALPHA .LT. ONEPT8) GAP = PT035                              GRID 058
      IF (ALPHA .LT. ONEPT6) GAP = PT04                               GRID 059
      IF (ALPHA .LT. ONEPT4) GAP = PT045                              GRID 060
      IF (ALPHA .LT. ONEPT2) GAP = PT025                              GRID 061
   40 TEMP = ZERO                                                     GRID 062
      DO 50 I = 1, INNER                                              GRID 063
      TEMP = TEMP + GAP                                               GRID 064
      PTS(I) = TEMP                                                   GRID 065
   50 CONTINUE                                                        GRID 066
C                                                                     GRID 067
C        LOGARITHMICALLY SPACE THE REST OF THE POINTS BY LOG(1 + U / 2) GRID 068
      TEMP = ALOG(ONE + TEMP/TWO)                                     GRID 069
      GAP = (ALOG(ONE + END/TWO) - TEMP) / FLOAT(NPTS2 - INNER)       GRID 070
      IND = INNER + 1                                                 GRID 071
      DO 60 I = IND, NPTS2                                            GRID 072
      TEMP = TEMP + GAP                                               GRID 073
      PTS(I) = TWO * (EXP(TEMP) - ONE)                                GRID 074
   60 CONTINUE                                                        GRID 075
      GO TO 100                                                       GRID 076
C                                                                     GRID 077
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C        CASE WHEN ALPHA .LE. 1 - SUBTRACT 1 FROM NO. OF INNER PTS      GRID 078
C        IF ALPHA .LE. 1/2.  START BY EQUISPACING ALL POINTS FOR        GRID 079
C        LOG(U + (MAX(ALPHA,0.3)**3), BUT MULTIPLY INNER POINTS BY      GRID 080
C        (MAX(ALPHA,0.3))**2 / 4.  (THE LATTER MULTIPLICATION IS        GRID 081
C        OMITTED IF KSUM .GT. 1.)  THEN CONTINUE SPACING.               GRID 082
   70 END = FIVE                                                        GRID 083
      IF (ALPHA .LT. ONE) END = FOUR                                    GRID 084
      IF (ALPHA .LT. PT9) END = FIVE                                    GRID 085
      IF (ALPHA .LT. PT8) END = SEVEN                                   GRID 086
      IF (ALPHA .LT. PT6) END = TEN                                     GRID 087
      AFAC1 = AMAX1(ALPHA,PT3)                                          GRID 088
      AFAC2 = ONE                                                       GRID 089
      IF (KSUM .EQ. 1) AFAC2 = AFAC1 * AFAC1 / FOUR                     GRID 090
      AFAC1 = AFAC1 * AFAC1 * AFAC1                                     GRID 091
      TEMP = ALOG(AFAC1)                                                GRID 092
      C1 = ALOG(END + AFAC1)                                            GRID 093
      GAP = (C1 - TEMP) / FLOAT(NPTS2)                                  GRID 094
      IF (ALPHA .LE. PT5) INNER = INNER - 1                             GRID 095
      DO 80 I = 1, INNER                                                GRID 096
      TEMP = TEMP + GAP                                                 GRID 097
      PTS(I) = (EXP(TEMP) - AFAC1) * AFAC2                              GRID 098
   80 CONTINUE                                                          GRID 099
      TEMP = ALOG(PTS(INNER) + AFAC1)                                   GRID 100
      GAP = (C1 - TEMP) / FLOAT(NPTS2 - INNER)                          GRID 101
      IND = INNER + 1                                                   GRID 102
      DO 90 I = IND, NPTS2                                              GRID 103
      TEMP = TEMP + GAP                                                 GRID 104
      PTS(I) = EXP(TEMP) - AFAC1                                        GRID 105
   90 CONTINUE                                                          GRID 106
C                                                                       GRID 107
C        COMPUTE WEIGHTS (ALL NPTS OF THEM).                            GRID 108
C        IF KSUM .GT. 1, ALL WEIGHTS ARE 1.                             GRID 109
  100 IF (KSUM .EQ. 1) GO TO 120                                        GRID 110
      DO 110 I = 1, NPTS                                                GRID 111
  110 WT(I) = ONE                                                       GRID 112
      RETURN                                                            GRID 113
C                                                                       GRID 114
  120 FLAG = MODE .NE. 0                                                GRID 115
      IND = NPTS2 + 1                                                   GRID 116
      DO 140 I = 1, NPTS2                                               GRID 117
      TEMP = PTS(I)                                                     GRID 118
      IND1 = NPTS2 + I                                                  GRID 119
      IND2 = IND - I                                                    GRID 120
      GAP = EXP(-XLAM*TEMP**ALPHA)                                      GRID 121
      IF (FLAG) GO TO 130                                               GRID 122
      WT(IND1) = GAP                                                    GRID 123
      WT(IND2) = GAP                                                    GRID 124
      GO TO 140                                                         GRID 125
  130 GAP = GAP * GAP                                                   GRID 126
      CALL CHARFN(TEMP, PAR, NPAR, END, AFAC1)                          GRID 127
      CALL CHARFN(TEMP + TEMP, PAR, NPAR, AFAC2, C1)                    GRID 128
      WT(IND1) = GAP / (ONE + TAU*(C1 - (END + AFAC1)**2))              GRID 129
      WT(IND2) = GAP / (ONE - TAU*(C1 + (END - AFAC1)**2))              GRID 130
  140 CONTINUE                                                          GRID 131
C                                                                       GRID 132
      RETURN                                                            GRID 133
      END                                                               GRID 134
C*********************************************************************CHAR 001
C        COMPUTES REAL AND IMAGINARY PARTS OF STANDARD STABLE           CHAR 002
C        CHARACTERISTIC FUNCTION (SIGMA = 1, MU = 0).                   CHAR 003
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C        CALLED BY - GRIDWT, SETECF, VARIAB                                    CHAR 004
C*************************************************************************CHAR 005
      SUBROUTINE CHARFN(U, PAR, NPAR, RE, XIM)                               CHAR 006
C        ARGUMENTS                                                           CHAR 007
      INTEGER NPAR                                                           CHAR 008
      REAL U, PAR(NPAR), RE, XIM                                             CHAR 009
C        LOCAL SCALARS                                                       CHAR 010
      REAL ALPHA, XMOD, ZERO, ONE, PIBY2                                     CHAR 011
      DATA ZERO, ONE, PIBY2 /0.0, 1.0, 1.570796327/                          CHAR 012
C                                                                            CHAR 013
      RE = ABS(U)                                                            CHAR 014
      ALPHA = PAR(1)                                                         CHAR 015
      IF (ALPHA .NE. ONE) GO TO 10                                           CHAR 016
      XIM = ZERO                                                             CHAR 017
      IF (U .NE. ZERO) XIM = ALOG(RE) / PIBY2                                CHAR 018
      GO TO 20                                                               CHAR 019
   10 XIM = TAN(PIBY2*ALPHA)                                                 CHAR 020
   20 XMOD = RE ** ALPHA                                                     CHAR 021
      XIM = -PAR(2) * SIGN(XMOD,U) * XIM                                     CHAR 022
      XMOD = EXP(-XMOD)                                                      CHAR 023
      RE = XMOD * COS(XIM)                                                   CHAR 024
      XIM = XMOD * SIN(XIM)                                                  CHAR 025
C                                                                            CHAR 026
      RETURN                                                                 CHAR 027
      END                                                                    CHAR 028
C*************************************************************************FUNC 001
C        FUNCTION/DERIVATIVE EVALUATION.                                     FUNC 002
C        CALLED BY - E04KBF, VARIAB, HESDIF                                  FUNC 003
C*************************************************************************FUNC 004
      SUBROUTINE FUNCT(IFLAG, N, XC, FC, GC, IW, LIW, W, LW)                 FUNC 005
C        ARGUMENTS                                                           FUNC 006
      INTEGER IFLAG, N, LIW, IW(LIW), LW                                     FUNC 007
      REAL XC(N), FC, GC(N), W(LW)                                           FUNC 008
C        LOCAL SCALARS                                                       FUNC 009
      LOGICAL ALF1, LFLAG                                                    FUNC 010
      INTEGER ILOW, NPTS, NPTS2, IND, IND1, ISUB, ISUB1, IPTS, IWT,          FUNC 011
     *IECF, IDERIV, IPSI                                                     FUNC 012
      REAL ALPHA, BSIGN, SIGMA, XMU, OMEGA, XMOD, PTSI, SINE, COSINE,        FUNC 013
     *PISEC2, SUEXP, XLOGSU, FAC, Z, Z1, ZERO, ONE, PIBY2                    FUNC 014
      DATA ZERO, ONE, PIBY2 /0.0, 1.0, 1.570796327/                          FUNC 015
C                                                                            FUNC 016
      ALPHA = XC(1)                                                          FUNC 017
      BSIGN = XC(2)                                                          FUNC 018
      SIGMA = XC(3)                                                          FUNC 019
      XMU = XC(4)                                                            FUNC 020
      ALF1 = ALPHA .EQ. ONE                                                  FUNC 021
      LFLAG = IFLAG .EQ. 0                                                   FUNC 022
C                                                                            FUNC 023
C        VARIABLES TO AID ADDRESSING IN W VECTOR - IPTS = ONE LESS THAN      FUNC 024
C        POSITION OF FIRST POSITIVE GRIDPOINT IN W VECTOR, ETC.              FUNC 025
      NPTS = IW(5)                                                           FUNC 026
      NPTS2 = NPTS / 2                                                       FUNC 027
      IND = NPTS + 1                                                         FUNC 028
      ILOW = NPTS2 + 1                                                       FUNC 029
      IPTS = IW(6)                                                           FUNC 030
      IWT = IPTS + NPTS2                                                     FUNC 031
      IECF = IWT + NPTS                                                      FUNC 032
      IDERIV = IECF + NPTS                                                   FUNC 033
      IPSI = IDERIV + N * NPTS                                               FUNC 034
      NPTS2 = IPTS - NPTS2                                                   FUNC 035
```

```
C        IF ALPHA.NE.1, COMPUTE OMEGA(U,ALPHA) AND ITS DERIVATIVE W. R.  FUNC 036
C        TO ALPHA OUTSIDE MAIN LOOP.                                    FUNC 037
      IF (ALF1) GO TO 10                                                FUNC 038
      OMEGA = TAN(PIBY2*ALPHA)                                          FUNC 039
      PISEC2 = PIBY2 * (ONE + OMEGA*OMEGA)                              FUNC 040
C                                                                       FUNC 041
C        LOOP OVER POSITIVE GRID PTS (SGN(U) IGNORED), SAVE PSI AND     FUNC 042
C        ITS GRADIENT AT ALL GRID PTS (PSI(U) = RE(PHI(U)) +            FUNC 043
C         IM(PHI(U)) - EMPIRICAL COUNTERPARTS.)                         FUNC 044
   10 DO 20 I = ILOW, NPTS                                              FUNC 045
      IND1 = IND - 1                                                    FUNC 046
      ISUB = NPTS2 + I                                                  FUNC 047
      PTSI = W(ISUB)                                                    FUNC 048
      XLOGSU = SIGMA * PTSI                                             FUNC 049
      SUEXP = XLOGSU ** ALPHA                                           FUNC 050
      XLOGSU = ALOG(XLOGSU)                                             FUNC 051
      IF (ALF1) OMEGA = XLOGSU / PIBY2                                  FUNC 052
      COSINE = XMU * PTSI - SUEXP * BSIGN * OMEGA                       FUNC 053
      SINE = SIN(COSINE)                                                FUNC 054
      COSINE = COS(COSINE)                                              FUNC 055
      XMOD = EXP(-SUEXP)                                                FUNC 056
      SUEXP = SUEXP * XMOD                                              FUNC 057
C                                                                       FUNC 058
C        SAVE COMPONENTS OF PSI                                         FUNC 059
      ISUB = IPSI + I                                                   FUNC 060
      ISUB1 = IECF + I                                                  FUNC 061
      W(ISUB) = XMOD * (COSINE + SINE) - W(ISUB1)                       FUNC 062
      ISUB = IPSI + IND1                                                FUNC 063
      ISUB1 = IECF + IND1                                               FUNC 064
      W(ISUB) = XMOD * (COSINE - SINE) - W(ISUB1)                       FUNC 065
      IF (LFLAG) GO TO 20                                               FUNC 066
C                                                                       FUNC 067
C        CALCULATE DERIVATIVES IF REQUIRED                              FUNC 068
C                                                                       FUNC 069
C        DERIVATIVES W. R. TO ALPHA                                     FUNC 070
      FAC = XLOGSU * OMEGA                                              FUNC 071
      IF ( .NOT. ALF1) FAC = FAC + PISEC2                               FUNC 072
      FAC = FAC * BSIGN                                                 FUNC 073
      Z = FAC + XLOGSU                                                  FUNC 074
      Z1 = FAC - XLOGSU                                                 FUNC 075
      ISUB = IDERIV + I                                                 FUNC 076
      W(ISUB) = SUEXP * (-Z*COSINE + Z1*SINE)                           FUNC 077
      ISUB1 = IDERIV + IND1                                             FUNC 078
      W(ISUB1) = SUEXP * (Z1*COSINE + Z*SINE)                           FUNC 079
C                                                                       FUNC 080
C        DERIVATIVES W. R. TO BETA                                      FUNC 081
      FAC = SUEXP * OMEGA                                               FUNC 082
      ISUB = ISUB + NPTS                                                FUNC 083
      W(ISUB) = FAC * (SINE - COSINE)                                   FUNC 084
      ISUB1 = ISUB1 + NPTS                                              FUNC 085
      W(ISUB1) = FAC * (SINE + COSINE)                                  FUNC 086
C                                                                       FUNC 087
C        DERIVATIVES W. R. TO SIGMA                                     FUNC 088
      FAC = BSIGN * OMEGA                                               FUNC 089
      Z = ONE + FAC                                                     FUNC 090
      Z1 = ONE - FAC                                                    FUNC 091
      FAC = -ALPHA * SUEXP / SIGMA                                      FUNC 092
      ISUB = ISUB + NPTS                                                FUNC 093
      W(ISUB) = FAC * (Z*COSINE + Z1*SINE)                              FUNC 094
      ISUB1 = ISUB1 + NPTS                                              FUNC 095
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      W(ISUB1) = FAC * (Z1*COSINE - Z*SINE)                              FUNC 096
C                                                                        FUNC 097
C        DERIVATIVES W. R. TO MU                                         FUNC 098
      FAC = PTSI * XMOD                                                  FUNC 099
      ISUB = ISUB + NPTS                                                 FUNC 100
      W(ISUB) = FAC * (-SINE + COSINE)                                   FUNC 101
      ISUB1 = ISUB1 + NPTS                                               FUNC 102
      W(ISUB1) = -FAC * (SINE + COSINE)                                  FUNC 103
   20 CONTINUE                                                           FUNC 104
C                                                                        FUNC 105
C        NOW COMPUTE OBJECTIVE FUNCTION , OPTIONALLY GRADIENT.           FUNC 106
      FC = ZERO                                                          FUNC 107
      IF (LFLAG) GO TO 40                                                FUNC 108
      ILOW = IDERIV - NPTS                                               FUNC 109
      DO 30 I = 1, N                                                     FUNC 110
   30 GC(I) = ZERO                                                       FUNC 111
   40 IF (IW(3) .EQ. 0) GO TO 70                                         FUNC 112
C                                                                        FUNC 113
C        SUM-OF-SQUARES ESTIMATION                                       FUNC 114
      DO 60 I = 1, NPTS                                                  FUNC 115
C        FN. EVALUATION                                                  FUNC 116
      ISUB = IPSI + I                                                    FUNC 117
      Z = W(ISUB)                                                        FUNC 118
      ISUB = IWT + I                                                     FUNC 119
      Z1 = Z * W(ISUB)                                                   FUNC 120
      FC = FC + Z * Z1                                                   FUNC 121
      IF (LFLAG) GO TO 60                                                FUNC 122
C        GRADIENT EVALUATION IF REQUESTED.                               FUNC 123
      ISUB = ILOW + I                                                    FUNC 124
      Z1 = Z1 + Z1                                                       FUNC 125
      DO 50 J = 1, N                                                     FUNC 126
      ISUB = ISUB + NPTS                                                 FUNC 127
      GC(J) = GC(J) + W(ISUB) * Z1                                       FUNC 128
   50 CONTINUE                                                           FUNC 129
   60 CONTINUE                                                           FUNC 130
      RETURN                                                             FUNC 131
C                                                                        FUNC 132
C        MATRIX ESTIMATION - FIRST MULTIPLY PSI VALUES BY WEIGHTS.       FUNC 133
   70 DO 80 I = 1, NPTS                                                  FUNC 134
      ISUB = IPSI + I                                                    FUNC 135
      ISUB1 = IWT + I                                                    FUNC 136
      W(ISUB) = W(ISUB) * W(ISUB1)                                       FUNC 137
   80 CONTINUE                                                           FUNC 138
C        POSITION OF A INVERSE IS REQUIRED.                              FUNC 139
      IND1 = IPSI + IND * NPTS                                           FUNC 140
      DO 110 I = 1, NPTS                                                 FUNC 141
      Z = ZERO                                                           FUNC 142
      IND1 = IND1 + NPTS                                                 FUNC 143
C        SUM OVER J OF PSI(J) * AINV(I,J)                                FUNC 144
      DO 90 J = 1, NPTS                                                  FUNC 145
      ISUB = IPSI + J                                                    FUNC 146
      ISUB1 = IND1 + J                                                   FUNC 147
      Z = Z + W(ISUB) * W(ISUB1)                                         FUNC 148
   90 CONTINUE                                                           FUNC 149
C        MULTIPLY BY PSI(I) AND ADD TO FN. VALUE                         FUNC 150
      ISUB = IPSI + I                                                    FUNC 151
      FC = FC + Z * W(ISUB)                                              FUNC 152
      IF (LFLAG) GO TO 110                                               FUNC 153
C                                                                        FUNC 154
C        GRADIENT IF REQUESTED - FOR JTH COMPONENT OF GRADIENT ADD       FUNC 155
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C        2*(JTH DERIVATIVE AT GRIDPOINT I)*WT(I)*(RESULT OF DO 90 LOOP) FUNC 156
      ISUB = IWT + I                                                    FUNC 157
      Z = (Z + Z) * W(ISUB)                                             FUNC 158
      ISUB = ILOW + I                                                   FUNC 159
      DO 100 J = 1, N                                                   FUNC 160
      ISUB = ISUB + NPTS                                                FUNC 161
      GC(J) = GC(J) + Z * W(ISUB)                                       FUNC 162
  100 CONTINUE                                                          FUNC 163
  110 CONTINUE                                                          FUNC 164
C                                                                       FUNC 165
      RETURN                                                            FUNC 166
      END                                                               FUNC 167
C*********************************************************************SETE 001
C        COMPUTES EMPIRICAL CH. F. VALUES, ADJUSTING FOR LOCATION,      SETE 002
C        SCALE, AND K-SUM INDEX.  FOR MATRIX ESTIMATION, THE UPPER      SETE 003
C        TRIANGLE OF A MATRIX IS CALCULATED AND INVERTED.               SETE 004
C        CALLED BY - STABLE                                             SETE 005
C        CALLS - CHARFN                                                 SETE 006
C        N.A.G. SUBROUTINE CALLED -                                     SETE 007
C               F01ABF (ACCURATE INVERSION OF POSITIVE DEFINITE         SETE 008
C               SYMMETRIC MATRIX).                                     SETE 009
C*********************************************************************SETE 010
      SUBROUTINE SETECF(X, N, PAR, NPAR, MODE, TAU, SIGMA, XMU, KSUM,   SETE 011
     *IA, NPTS2, NPTS, PTS, ECF, A, AINV, WORK, IFAULT)                 SETE 012
C        ARGUMENTS                                                      SETE 013
      INTEGER N, NPAR, MODE, KSUM, IA, NPTS2, NPTS, IFAULT              SETE 014
      REAL X(N), PAR(NPAR), TAU, SIGMA, XMU, PTS(NPTS2), ECF(NPTS),     SETE 015
     *A(IA,NPTS), AINV(NPTS,NPTS), WORK(NPTS)                           SETE 016
C        LOCAL SCALARS                                                  SETE 017
      INTEGER IND, IND1, IND2, IND3                                     SETE 018
      REAL PTSI, PTSJ, RE, XIM, RE1, XIM1, RPI, RMI, RPI1, RMI1, ZERO,  SETE 019
     *HALF                                                              SETE 020
      DATA ZERO, HALF /0.0, 0.5/                                        SETE 021
C                                                                       SETE 022
C        CALCULATION OF E.CH.F. VALUES                                  SETE 023
      PTSJ = FLOAT(N)                                                   SETE 024
      XIM1 = FLOAT(KSUM)                                                SETE 025
      RPI = XIM1 * HALF                                                 SETE 026
      IND = NPTS2 + 1                                                   SETE 027
      IND1 = NPTS + 1                                                   SETE 028
      DO 20 I = IND, NPTS                                               SETE 029
      IND2 = I - NPTS2                                                  SETE 030
      PTSI = PTS(IND2) / SIGMA                                          SETE 031
      IND2 = IND1 - I                                                   SETE 032
      RE = ZERO                                                         SETE 033
      XIM = ZERO                                                        SETE 034
C                                                                       SETE 035
      DO 10 J = 1, N                                                    SETE 036
      RPI1 = X(J) * PTSI                                                SETE 037
      RE = RE + COS(RPI1)                                               SETE 038
      XIM = XIM + SIN(RPI1)                                             SETE 039
   10 CONTINUE                                                          SETE 040
C                                                                       SETE 041
      RE = RE / PTSJ                                                    SETE 042
      XIM = XIM / PTSJ                                                  SETE 043
      RMI = (RE*RE + XIM*XIM) ** RPI                                    SETE 044
      RPI1 = XIM1 * ATAN2(XIM,RE) - XMU * PTSI                          SETE 045
      RE = RMI * COS(RPI1)                                              SETE 046
      XIM = RMI * SIN(RPI1)                                             SETE 047
      ECF(I) = RE + XIM                                                 SETE 048
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      ECF(IND2) = RE - XIM                                                SETE 049
   20 CONTINUE                                                            SETE 050
C                                                                         SETE 051
C        SET UPPER TRIANGLE OF A IF REQUESTED.  A GENERATED FROM          SETE 052
C        POSITIVE GRIDPOINTS ONLY - ANTIDIAGONAL COMPUTED TWICE.          SETE 053
      IF (MODE .NE. 0) RETURN                                             SETE 054
C        FIRST FILL WORK WITH (RE + IM) (PHI) TO SAVE EVALS.              SETE 055
      DO 30 I = IND, NPTS                                                 SETE 056
      IND2 = I - NPTS2                                                    SETE 057
      CALL CHARFN(PTS(IND2), PAR, NPAR, RE, XIM)                          SETE 058
      IND2 = IND1 - I                                                     SETE 059
      WORK(I) = RE + XIM                                                  SETE 060
      WORK(IND2) = RE - XIM                                               SETE 061
   30 CONTINUE                                                            SETE 062
C        COMPUTATION OF A.                                                SETE 063
      DO 40 I = IND, NPTS                                                 SETE 064
      IND2 = I - NPTS2                                                    SETE 065
      PTSI = PTS(IND2)                                                    SETE 066
      IND2 = IND1 - I                                                     SETE 067
      RPI = WORK(I)                                                       SETE 068
      RMI = WORK(IND2)                                                    SETE 069
      DO 40 J = IND, I                                                    SETE 070
      IND3 = J - NPTS2                                                    SETE 071
      PTSJ = PTS(IND3)                                                    SETE 072
      IND3 = IND1 - J                                                     SETE 073
      RPI1 = WORK(J)                                                      SETE 074
      RMI1 = WORK(IND3)                                                   SETE 075
      CALL CHARFN(PTSI + PTSJ, PAR, NPAR, RE, XIM)                        SETE 076
      CALL CHARFN(PTSI - PTSJ, PAR, NPAR, RE1, XIM1)                      SETE 077
      A(J,I) = RE1 + XIM - RPI * RPI1                                     SETE 078
      A(IND2,J) = RE - XIM1 - RMI * RPI1                                  SETE 079
      A(IND3,I) = RE + XIM1 - RPI * RMI1                                  SETE 080
      A(IND2,IND3) = RE1 - XIM - RMI * RMI1                               SETE 081
   40 CONTINUE                                                            SETE 082
C                                                                         SETE 083
C        DIAGONAL OF A ADDITIVELY INFLATED BY TAU TIMES AVERAGE OF        SETE 084
C        DIAGONAL ELEMENTS.                                               SETE 085
      IF (TAU .EQ. ZERO) GO TO 70                                         SETE 086
      PTSI = ZERO                                                         SETE 087
      DO 50 I = 1, NPTS                                                   SETE 088
   50 PTSI = PTSI + A(I,I)                                                SETE 089
      PTSI = TAU * PTSI / FLOAT(NPTS)                                     SETE 090
      DO 60 I = 1, NPTS                                                   SETE 091
   60 A(I,I) = A(I,I) + PTSI                                              SETE 092
C                                                                         SETE 093
C        INVERT A USING N.A.G. ROUTINE F01ABF                             SETE 094
   70 IFAULT = 1                                                          SETE 095
      CALL F01ABF(A, IA, NPTS, AINV, NPTS, WORK, IFAULT)                  SETE 096
C        EXIT IF A FOUND NON POSITIVE DEFINITE OR ILL-CONDITIONED.        SETE 097
      IF (IFAULT .GT. 0) RETURN                                           SETE 098
C        ARRANGE A INVERSE SO IT IS COMPLETELY FILLED.                    SETE 099
      DO 80 I = 1, NPTS                                                   SETE 100
      DO 80 J = 1, I                                                      SETE 101
      AINV(J,I) = AINV(I,J)                                               SETE 102
   80 CONTINUE                                                            SETE 103
C                                                                         SETE 104
      RETURN                                                              SETE 105
      END                                                                 SETE 106
C*************************************************************************MON1 001
C     MONITORING OF E04KBF.                                               MON1 002
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C       CALLED BY - E04KBF                                                      MONI 003
C*********************************************************************************MONI 004
      SUBROUTINE MONIT(N, XC, FC, GC, ISTATE, GPJNRM, COND, POSDEF,             MONI 005
     *NITER, NF, IW, LIW, W, LW)                                                MONI 006
C        ARGUMENTS                                                              MONI 007
      LOGICAL POSDEF                                                            MONI 008
      INTEGER N, ISTATE(N), NITER, NF, LIW, IW(LIW), LW                         MONI 009
      REAL XC(N), FC, GC(N), GPJNRM, COND, W(LW)                                MONI 010
C        LOCAL SCALAR                                                           MONI 011
      INTEGER IUNIT                                                             MONI 012
C                                                                               MONI 013
C        STORE HESSIAN CONDITION NUMBER AND PROJECTED GRADIENT NORM IN          MONI 014
C        WORK VECTOR                                                            MONI 015
      IUNIT = 9 * N + 1                                                         MONI 016
      W(IUNIT) = COND                                                           MONI 017
      W(IUNIT + 1) = GPJNRM                                                     MONI 018
      IUNIT = IW(4)                                                             MONI 019
      IF (IUNIT .LE. 0) RETURN                                                  MONI 020
C                                                                               MONI 021
C        WRITE DETAILS OF OPTIMIZATION PROCESS IF IUNIT .GT. 0                  MONI 022
      WRITE (IUNIT,10) NITER, NF, FC, GPJNRM                                    MONI 023
      WRITE (IUNIT,20) (XC(I),I=1,N)                                            MONI 024
      WRITE (IUNIT,30) (GC(I),I=1,N)                                            MONI 025
      WRITE (IUNIT,40) COND                                                     MONI 026
C                                                                               MONI 027
   10 FORMAT (5HOITNS, 5X, 8HFN EVALS, 8X, 8HFN VALUE, 5X,                      MONI 028
     *21HNORM OF PROJ GRADIENT/1H , I4, 8X, I5, 5X, E11.4, 15X, E11.4)          MONI 029
   20 FORMAT (10HOSOLUTIONS, 4E13.5)                                            MONI 030
   30 FORMAT (10H PROJ GRAD, 4E13.5)                                            MONI 031
   40 FORMAT (50H ESTIMATED CONDITION NUMBER OF PROJECTED HESSIAN =,             MONI 032
     *E12.2)                                                                    MONI 033
      RETURN                                                                    MONI 034
      END                                                                       MONI 035
C*********************************************************************************VARI 001
C        CALCULATES EMPIRICAL (VCV1) AND ASYMPTOTIC (VCV2)                      VARI 002
C        APPROXIMATIONS TO ASYMPTOTIC COVARIANCE MATRICES.  IFAIL1 AND          VARI 003
C        IFAIL2 ARE FAILURE INDICATORS FOR MATRIX INVERSION REQUIRED            VARI 004
C        FOR VCV1, VCV2 RESPECTIVELY.                                           VARI 005
C        CALLED BY - STABLE                                                     VARI 006
C        CALLS - HESDIF, FUNCT, CHARFN, SETVCV, VMATRX, DAPROD, HVPROD          VARI 007
C        N.A.G. SUBROUTINES CALLED -                                            VARI 008
C               F01CAF (SETS A MATRIX TO ZERO),                                 VARI 009
C               F01CMF (SET ONE MATRIX TO ANOTHER).                             VARI 010
C*********************************************************************************VARI 011
      SUBROUTINE VARIAB(ICOV, X, N, PAR, NPAR, MODE, SIGMA, XMU, ISUB,          VARI 012
     *NVAR, PTS, NPTS2, WT, ECF, NPTS, DERIV, WORK, HOLD, A, IA, AINV,          VARI 013
     *VCV1, VCV2, H, NVAR1, V, IW, LIW, W, LW, IFAIL1, IFAIL2)                  VARI 014
C        ARGUMENTS                                                              VARI 015
      INTEGER ICOV, N, NPAR, MODE, NVAR, ISUB(NVAR), NPTS2, NPTS, IA,           VARI 016
     *NVAR1, LIW, IW(LIW), LW, IFAIL1, IFAIL2                                   VARI 017
      REAL X(N), PAR(NPAR), SIGMA, XMU, PTS(NPTS2), WT(NPTS), ECF(NPTS),VARI 018
     *DERIV(NPTS,NPAR), WORK(NPTS), HOLD(NVAR), A(IA,NPTS),                     VARI 019
     *AINV(NPTS,NPTS), VCV1(NPAR,NPAR), VCV2(NPAR,NPAR), H(NVAR1,NVAR),         VARI 020
     *V(NVAR,NVAR), W(LW)                                                       VARI 021
C        LOCAL SCALARS                                                          VARI 022
      LOGICAL FLAG                                                              VARI 023
      INTEGER IND, IND1, IND2, IND3                                             VARI 024
      REAL PTSK, PTSL, RPI, RMI, RPI1, RMI1, COVKL, COVML, COVKM, COVMM,VARI 025
     *D1, D2, D3, D4, ZERO                                                      VARI 026
      DATA ZERO /0.0/                                                           VARI 027
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C                                                                       VARI 028
      IND = NPTS2 + 1                                                   VARI 029
      IND1 = NPTS + 1                                                   VARI 030
C                                                                       VARI 031
C        IF REQUESTED, FIRST CALCULATE HESSIAN FOR EMPIRICAL VERSION    VARI 032
C        AND STORE IN VCV1.  (HESDIF, FUNCT REQUIRE ECF, WORK,          VARI 033
C        POSSIBLY AINV, WHICH ARE USED AS WORK AREAS BELOW.)            VARI 034
C        H AND V ARE PASSED AS WORKSPACE.                               VARI 035
      IF (ICOV .EQ. 0) CALL HESDIF(PAR, NPAR, ISUB, VCV1, H, V, NVAR,   VARI 036
     *IW, LIW, W, LW)                                                   VARI 037
C                                                                       VARI 038
C        CALL FUNCT TO SET DERIV, AS GRID SEARCH PERFORMED BY E04KBF    VARI 039
C        MAY HAVE SET IT TO STRANGE VALUES.  VCV2 USED AS WORKSPACE.    VARI 040
      CALL FUNCT(2, NPAR, PAR, D1, VCV2(1,1), IW, LIW, W, LW)           VARI 041
C                                                                       VARI 042
C        SHIFT DERIV VALUES SO THEY CAN BE ADDRESSED WITHOUT THE        VARI 043
C        ISUB VECTOR.  NOTE ISUB ELEMENTS ARE IN ASCENDING ORDER.       VARI 044
      DO 20 I = 1, NVAR                                                 VARI 045
      IND2 = ISUB(I)                                                    VARI 046
      IF (IND2 .EQ. I) GO TO 20                                         VARI 047
      DO 10 J = 1, NPTS                                                 VARI 048
   10 DERIV(J,I) = DERIV(J,IND2)                                        VARI 049
   20 CONTINUE                                                          VARI 050
C                                                                       VARI 051
C        FILL ECF VECTOR WITH CH. F. VALUES, NOW THAT IT IS NO          VARI 052
C        LONGER NEEDED FOR FUNCTION EVALUATION.                         VARI 053
      DO 30 I = IND, NPTS                                               VARI 054
      IND2 = I - NPTS2                                                  VARI 055
      CALL CHARFN(PTS(IND2), PAR, NPAR, D1, D2)                         VARI 056
      IND2 = IND1 - I                                                   VARI 057
      ECF(I) = D1 + D2                                                  VARI 058
      ECF(IND2) = D1 - D2                                               VARI 059
   30 CONTINUE                                                          VARI 060
      IF (MODE .EQ. 0) GO TO 100                                        VARI 061
C                                                                       VARI 062
C        SUM OF SQUARES ESTIMATION SECTION.                             VARI 063
C                                                                       VARI 064
C        FIRST DO ASYMPTOTIC VERSION.                                   VARI 065
C        CALCULATE UPPER TRIANGLE OF HESSIAN.                           VARI 066
      DO 50 I = 1, NVAR                                                 VARI 067
      DO 50 J = I, NVAR                                                 VARI 068
      D1 = ZERO                                                         VARI 069
      DO 40 K = 1, NPTS                                                 VARI 070
   40 D1 = D1 + DERIV(K,I) * DERIV(K,J) * WT(K)                         VARI 071
      H(I,J) = D1                                                       VARI 072
   50 CONTINUE                                                          VARI 073
C                                                                       VARI 074
C        PREMULTIPLY DERIV BY WEIGHTS TO SAVE MULTIPLICATIONS.          VARI 075
      DO 60 I = 1, NPTS                                                 VARI 076
      D1 = WT(I)                                                        VARI 077
      DO 60 J = 1, NVAR                                                 VARI 078
      DERIV(I,J) = D1 * DERIV(I,J)                                      VARI 079
   60 CONTINUE                                                          VARI 080
C                                                                       VARI 081
C        COMPUTE UPPER TRIANGLE OF V.  BASICALLY EQUIVALENT TO          VARI 082
C        CALCULATING THE A MATRIX FOR MATRIX ESTIMATION, BUT            VARI 083
C        COMPLICATIONS ARISE IN COMPUTING BILINEAR FORMS.               VARI 084
      CALL F01CAF(V, NVAR, NVAR, IFAIL2)                                VARI 085
      DO 90 K = IND, NPTS                                               VARI 086
      IND2 = K - NPTS2                                                  VARI 087
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      PTSK = PTS(IND2)                                                  VARI 088
      IND2 = IND1 - K                                                   VARI 089
      RPI = ECF(K)                                                      VARI 090
      RMI = ECF(IND2)                                                   VARI 091
      DO 90 L = IND, K                                                  VARI 092
      IND3 = L - NPTS2                                                  VARI 093
      PTSL = PTS(IND3)                                                  VARI 094
      IND3 = IND1 - L                                                   VARI 095
      RPI1 = ECF(L)                                                     VARI 096
      RMI1 = ECF(IND3)                                                  VARI 097
      CALL CHARFN(PTSK + PTSL, PAR, NPAR, D1, D2)                       VARI 098
      CALL CHARFN(PTSK - PTSL, PAR, NPAR, D3, D4)                       VARI 099
      COVKL = D3 + D2 - RPI * RPI1                                      VARI 100
      COVML = D1 - D4 - RMI * RPI1                                      VARI 101
      COVKM = D1 + D4 - RPI * RMI1                                      VARI 102
      COVMM = D3 - D2 - RMI * RMI1                                      VARI 103
      FLAG = K .EQ. L                                                   VARI 104
C        LOOP TO ADD CONTRIBUTIONS TO V (BILINEAR FORMS).               VARI 105
      DO 80 I = 1, NVAR                                                 VARI 106
      D1 = DERIV(K,I)                                                   VARI 107
      D2 = DERIV(IND2,I)                                                VARI 108
      DO 80 J = 1, NVAR                                                 VARI 109
      D3 = DERIV(L,J)                                                   VARI 110
      D4 = DERIV(IND3,J)                                                VARI 111
      PTSL = (COVKL*D1 + COVML*D2) * D3 + (COVKM*D1 + COVMM*D2) * D4    VARI 112
      IF (FLAG) GO TO 70                                                VARI 113
C                                                                       VARI 114
C        WHEN K .NE. L , MUST ADD SYMMETRIC CONTRIBUTION.               VARI 115
      RPI1 = DERIV(K,J)                                                 VARI 116
      RMI1 = DERIV(IND2,J)                                              VARI 117
      D3 = DERIV(L,I)                                                   VARI 118
      D4 = DERIV(IND3,I)                                                VARI 119
      PTSL = PTSL + (COVKL*RPI1 + COVML*RMI1) * D3 + (COVKM*RPI1 +      VARI 120
     *COVMM*RMI1) * D4                                                  VARI 121
   70 V(I,J) = V(I,J) + PTSL      .                                     VARI 122
   80 CONTINUE                                                          VARI 123
   90 CONTINUE                                                          VARI 124
      GO TO 140                                                         VARI 125
C                                                                       VARI 126
C        MATRIX ESTIMATION SECTION.                                     VARI 127
C                                                                       VARI 128
C        FILL A MATRIX COMPLETELY (UPPER TRIANGLE ONLY ON ENTRY),       VARI 129
C        MULTIPLY ELEMENTS OF A BY CORRESPONDING WEIGHTS, MULTIPLY      VARI 130
C        DERIV VALUES BY WEIGHTS TO SAVE MULTIPLICATIONS LATER.         VARI 131
  100 DO 130 I = 1, NPTS                                                VARI 132
      D1 = WT(I)                                                        VARI 133
      DO 110 J = I, NPTS                                                VARI 134
      A(I,J) = A(I,J) * D1 * WT(J)                                      VARI 135
      A(J,I) = A(I,J)                                                   VARI 136
  110 CONTINUE                                                          VARI 137
      DO 120 J = 1, NVAR                                                VARI 138
  120 DERIV(I,J) = DERIV(I,J) * D1                                      VARI 139
  130 CONTINUE                                                          VARI 140
C                                                                       VARI 141
C        ASYMPTOTIC VERSION.                                            VARI 142
C        MULTIPLY AINV * DERIV, OVERWRITING CORNER OF AINV AND USING    VARI 143
C        HOLD AS WORKSPACE.                                             VARI 144
      CALL DAPROD(AINV, NPTS, NPTS, DERIV, HOLD, NVAR)                  VARI 145
C                                                                       VARI 146
C        MULTIPLY A * (AINV CORNER), OVERWRITING CORNER OF A AND        VARI 147
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```
      DO 50 I = 1, N                                                    VMAT 030
      D1 = (X(I) - XMU) / SIGMA                                         VMAT 031
C                                                                       VMAT 032
C        WORK HOLDS VECTOR OF SINE/COSINE TERMS.                        VMAT 033
      DO 10 J = IND, NPTS                                               VMAT 034
      IND2 = J - NPTS2                                                  VMAT 035
      D2 = PTS(IND2) * D1                                               VMAT 036
      D3 = COS(D2)                                                      VMAT 037
      D2 = SIN(D2)                                                      VMAT 038
      IND2 = IND1 - J                                                   VMAT 039
      WORK(J) = ECF(J) - D3 - D2                                        VMAT 040
      WORK(IND2) = ECF(IND2) - D3 + D2                                  VMAT 041
      IF (FLAG) GO TO 10                                                VMAT 042
C                                                                       VMAT 043
C        IF MATRIX ESTIMATION, MULTIPLY ELEMENTS OF WORK BY WEIGHTS.    VMAT 044
      WORK(J) = WORK(J) * WT(J)                                         VMAT 045
      WORK(IND2) = WORK(IND2) * WT(IND2)                                VMAT 046
   10 CONTINUE                                                          VMAT 047
C                                                                       VMAT 048
C        MULTIPLY DERIV * WORK, WRITING RESULT TO HOLD.  MULTIPLICATION VMAT 049
C        DONE DIRECTLY TO AVOID OVERHEAD OF SUBROUTINE CALL.            VMAT 050
      DO 30 J = 1, NVAR                                                 VMAT 051
      D1 = ZERO                                                         VMAT 052
      DO 20 K = 1, NPTS                                                 VMAT 053
   20 D1 = D1 + DERIV(K,J) * WORK(K)                                    VMAT 054
      HOLD(J) = D1                                                      VMAT 055
   30 CONTINUE                                                          VMAT 056
C                                                                       VMAT 057
C        ADD HOLD * (HOLD TRANSPOSE) TO V.                              VMAT 058
      DO 40 J = 1, NVAR                                                 VMAT 059
      D1 = HOLD(J)                                                      VMAT 060
      DO 40 K = J, NVAR                                                 VMAT 061
      V(J,K) = V(J,K) + D1 * HOLD(K)                                    VMAT 062
   40 CONTINUE                                                          VMAT 063
   50 CONTINUE                                                          VMAT 064
C                                                                       VMAT 065
C        FINAL CONSTANT FACTOR FOR V.                                   VMAT 066
      D1 = FOUR / FLOAT(N)                                              VMAT 067
      DO 60 I = 1, NVAR                                                 VMAT 068
      DO 60 J = I, NVAR                                                 VMAT 069
   60 V(I,J) = V(I,J) * D1                                              VMAT 070
C                                                                       VMAT 071
      RETURN                                                            VMAT 072
      END                                                               VMAT 073
C*************************************************************************DAPR 001
C        MULTIPLIES THE (NPTS BY NPTS) CORNER OF THE (IFAC1 BY NPTS)    DAPR 002
C        MATRIX FAC1 BY THE (NPTS BY NVAR) MATRIX FAC2, OVERWRITING     DAPR 003
C        THE UPPER LEFT (NPTS BY NVAR) ELEMENTS OF FAC1.                DAPR 004
C        UNFORTUNATELY, N.A.G. ROUTINE F01CKF DOES NOT ALLOW THIS       DAPR 005
C        KIND OF OVERWRITING.                                           DAPR 006
C        CALLED BY - VARIAB                                             DAPR 007
C*************************************************************************DAPR 008
      SUBROUTINE DAPROD(FAC1, IFAC1, NPTS, FAC2, WORK, NVAR)            DAPR 009
C        ARGUMENTS                                                      DAPR 010
      INTEGER IFAC1, NPTS, NVAR                                         DAPR 011
      REAL FAC1(IFAC1,NPTS), FAC2(NPTS,NVAR), WORK(NVAR)                DAPR 012
C        LOCAL SCALARS                                                  DAPR 013
      REAL TEMP, ZERO                                                   DAPR 014
      DATA ZERO /0.0/                                                   DAPR 015
C                                                                       DAPR 016
```

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C        USING HOLD AS WORKSPACE.                                              VARI 148
      CALL DAPROD(A, IA, NPTS, AINV, HOLD, NVAR)                               VARI 149
C                                                                              VARI 150
C        MULTIPLY (A CORNER TRANSPOSE) * (AINV CORNER), GIVING                 VARI 151
C        UPPER TRIANGLE OF V.                                                  VARI 152
      CALL HVPROD(A, IA, NVAR, AINV, NPTS, V, NVAR)                            VARI 153
C                                                                              VARI 154
C        MULTIPLY (AINV CORNER TRANSPOSE) * DERIV, GIVING UPPER                VARI 155
C        TRIANGLE OF HESSIAN.                                                  VARI 156
      CALL HVPROD(AINV, NPTS, NVAR, DERIV, NPTS, H, NVAR1)                     VARI 157
C                                                                              VARI 158
C        CODE COMMON TO MATRIX AND SUM OF SQUARES ESTIMATION.                  VARI 159
C        COMPUTE ASYMPTOTIC COVARIANCE MATRIX.                                 VARI 160
  140 CALL SETVCV(ISUB, NVAR, H, NVAR1, V, HOLD, VCV2, NPAR, SIGMA,            VARI 161
     *IFAIL2)                                                                  VARI 162
      IF (ICOV .GT. 0) RETURN                                                  VARI 163
C                                                                              VARI 164
C        EMPIRICAL VERSION IF REQUESTED.                                       VARI 165
C        COMPUTE EMPIRICAL V MATRIX, USING WORK AND HOLD AS WORK AREAS.        VARI 166
      IF (MODE .NE. 0) CALL VMATRX(X, N, MODE, XMU, SIGMA, PTS, NPTS2,         VARI 167
     *WT, ECF, WORK, NPTS, DERIV, V, HOLD, NVAR)                               VARI 168
      IF (MODE .EQ. 0) CALL VMATRX(X, N, MODE, XMU, SIGMA, PTS, NPTS2,         VARI 169
     *WT, ECF, WORK, NPTS, AINV, V, HOLD, NVAR)                                VARI 170
C                                                                              VARI 171
C        RESTORE HESSIAN FROM VCV1, COMPUTE COVARIANCE MATRIX.                 VARI 172
      CALL F01CHF(VCV1, NVAR, H, NVAR1, NVAR, NVAR)                            VARI 173
      CALL SETVCV(ISUB, NVAR, H, NVAR1, V, HOLD, VCV1, NPAR, SIGMA,            VARI 174
     *IFAIL1)                                                                  VARI 175
C                                                                              VARI 176
      RETURN                                                                   VARI 177
      END                                                                      VARI 178
C*************************************************************************VMAT 001
C        CALCULATES EMPIRICAL V MATRIX.  IMPLICIT IS COMPUTATION OF            VMAT 002
C        EMPIRICAL COVARIANCE KERNEL, BUT IT IS FASTER TO COMPUTE A            VMAT 003
C        MATRIX PRODUCT FOR EACH SAMPLE POINT THAN TO CUMULATE THE             VMAT 004
C        WHOLE KERNEL.  FOR MATRIX ESTIMATION, THE DERIV ARRAY                 VMAT 005
C        IS ACTUALLY THE UPPER LEFT CORNER OF AINV.                            VMAT 006
C        CALLED BY - VARIAB                                                    VMAT 007
C        N.A.G. SUBROUTINE CALLED -                                            VMAT 008
C                F01CAF (SET A MATRIX TO 0).                                   VMAT 009
C*************************************************************************VMAT 010
      SUBROUTINE VMATRX(X, N, MODE, XMU, SIGMA, PTS, NPTS2, WT, ECF,           VMAT 011
     *WORK, NPTS, DERIV, V, HOLD, NVAR)                                        VMAT 012
C        ARGUMENTS                                                             VMAT 013
      INTEGER N, MODE, NPTS2, NPTS, NVAR                                       VMAT 014
      REAL X(N), XMU, SIGMA, PTS(NPTS2), WT(NPTS), ECF(NPTS),                  VMAT 015
     *WORK(NPTS), DERIV(NPTS,NVAR), V(NVAR,NVAR), HOLD(NVAR)                   VMAT 016
C        LOCAL SCALARS                                                         VMAT 017
      LOGICAL FLAG                                                             VMAT 018
      INTEGER IND, IND1, IND2                                                  VMAT 019
      REAL D1, D2, D3, ZERO, FOUR                                              VMAT 020
      DATA ZERO, FOUR /0.0, 4.0/                                               VMAT 021
C                                                                              VMAT 022
C        SET V TO 0.                                                           VMAT 023
      FLAG = MODE .NE. 0                                                       VMAT 024
      IND = NPTS2 + 1                                                          VMAT 025
      IND1 = NPTS + 1                                                          VMAT 026
      CALL F01CAF(V, NVAR, NVAR, IND2)                                         VMAT 027
C                                                                              VMAT 028
C        MAIN LOOP OVER SAMPLE.                                                VMAT 029
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      DO 40 I = 1, NPTS                                                 DAPR 017
      DO 20 J = 1, NVAR                                                 DAPR 018
      TEMP = ZERO                                                       DAPR 019
      DO 10 K = 1, NPTS                                                 DAPR 020
   10 TEMP = TEMP + FAC1(I,K) * FAC2(K,J)                               DAPR 021
      WORK(J) = TEMP                                                    DAPR 022
   20 CONTINUE                                                          DAPR 023
      DO 30 J = 1, NVAR                                                 DAPR 024
   30 FAC1(I,J) = WORK(J)                                               DAPR 025
   40 CONTINUE                                                          DAPR 026
C                                                                       DAPR 027
      RETURN                                                            DAPR 028
      END                                                               DAPR 029
C*********************************************************************HVPR 001
C        MULTIPLIES THE TRANSPOSED (NPTS BY NVAR) CORNER OF THE         HVPR 002
C        (IFAC1 BY NVAR) MATRIX FAC1 BY THE (NPTS BY NVAR) MATRIX       HVPR 003
C        FAC2, GIVING THE UPPER TRIANGLE OF EITHER V OR H.              HVPR 004
C        CALLED BY - VARIAB                                             HVPR 005
C*********************************************************************HVPR 006
      SUBROUTINE HVPROD(FAC1, IFAC1, NVAR, FAC2, NPTS, VH, IVH)         HVPR 007
C        ARGUMENTS                                                      HVPR 008
      INTEGER IFAC1, NVAR, NPTS, IVH                                    HVPR 009
      REAL FAC1(IFAC1,NVAR), FAC2(NPTS,NVAR), VH(IVH,NVAR)              HVPR 010
C        LOCAL SCALARS                                                  HVPR 011
      REAL TEMP, ZERO                                                   HVPR 012
      DATA ZERO /0.0/                                                   HVPR 013
C                                                                       HVPR 014
      DO 20 I = 1, NVAR                                                 HVPR 015
      DO 20 J = I, NVAR                                                 HVPR 016
      TEMP = ZERO                                                       HVPR 017
      DO 10 K = 1, NPTS                                                 HVPR 018
   10 TEMP = TEMP + FAC1(K,I) * FAC2(K,J)                               HVPR 019
      VH(I,J) = TEMP                                                    HVPR 020
   20 CONTINUE                                                          HVPR 021
C                                                                       HVPR 022
      RETURN                                                            HVPR 023
      END                                                               HVPR 024
C*********************************************************************SETV 001
C        COMMON OPERATIONS IN COMPUTATION OF COVARIANCE MATRICES.       SETV 002
C        INVERTS HESSIAN MATRIX H, CALCULATES (H INVERSE) * V *         SETV 003
C        (H INVERSE), OVERWRITING V.                                    SETV 004
C        CALLED BY - VARIAB                                             SETV 005
C        N.A.G. SUBROUTINES CALLED -                                    SETV 006
C               F01ABF (ACCURATE INVERSION OF POSITIVE DEFINITE         SETV 007
C                       SYMMETRIC MATRIX),                              SETV 008
C               F01CKF (MATRIX MULTIPLICATION WITH OVERWRITING),        SETV 009
C               F01CMF (SET ONE MATRIX EQUAL TO ANOTHER),               SETV 010
C               F01CAF (SET A MATRIX TO ZERO).                          SETV 011
C*********************************************************************SETV 012
      SUBROUTINE SETVCV(ISUB, NVAR, H, NVAR1, V, WORK, VCV, NPAR, SIGMA,SETV 013
     *IFAULT)                                                           SETV 014
C        ARGUMENTS                                                      SETV 015
      INTEGER NVAR, ISUB(NVAR), NVAR1, NPAR, IFAULT                     SETV 016
      REAL H(NVAR1,NVAR), V(NVAR,NVAR), WORK(NVAR), VCV(NPAR,NPAR),     SETV 017
     *SIGMA                                                             SETV 018
C        LOCAL SCALARS                                                  SETV 019
      INTEGER IND, IND1                                                 SETV 020
      REAL TEMP, ZERO                                                   SETV 021
      DATA ZERO /0.0/                                                   SETV 022
C                                                                       SETV 023
```

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C        INVERT H, USING VCV AS WORKSPACE.                                    SETV 024
      IFAULT = 1                                                              SETV 025
      CALL F01ABF(H, NVAR1, NVAR, VCV, NPAR, WORK, IFAULT)                    SETV 026
      IF (IFAULT .EQ. 0) GO TO 10                                             SETV 027
C        ON FAILURE OF INVERSION, SET VCV TO 0 AND RETURN.                    SETV 028
      CALL F01CAF(VCV, NPAR, NPAR, IND)                                       SETV 029
      RETURN                                                                  SETV 030
C        FILL OUT VCV AND V (CURRENTLY ONLY HALF FULL).                       SETV 031
   10 DO 20 I = 1, NVAR                                                       SETV 032
      DO 20 J = 1, I                                                          SETV 033
      V(I,J) = V(J,I)                                                         SETV 034
      VCV(J,I) = VCV(I,J)                                                     SETV 035
   20 CONTINUE                                                                SETV 036
C                                                                             SETV 037
C        SET H TO ITS INVERSE IN SUCH A WAY THAT MULTIPLICATION VIA           SETV 038
C        F01CKF WILL BE CORRECT.  (NOTE DIMENSIONS IN F01CMF CALL)            SETV 039
      CALL F01CMF(VCV, NPAR, H, NVAR, NVAR, NVAR)                             SETV 040
C                                                                             SETV 041
C        MULTIPLY H * V, OVERWRITING V.                                       SETV 042
      CALL F01CKF(V, H, V, NVAR, NVAR, NVAR, WORK, NVAR, 3, IFAULT)           SETV 043
C                                                                             SETV 044
C        MULTIPLY V * H, OVERWRITING V.                                       SETV 045
      CALL F01CKF(V, V, H, NVAR, NVAR, NVAR, WORK, NVAR, 2, IFAULT)           SETV 046
C                                                                             SETV 047
C        V NOW CONTAINS COVARIANCE MATRIX FOR FREE VARIABLES.  ARRANGE        SETV 048
C        ITS CONTENTS IN VCV, ADJUST SIGMA AND MU ENTRIES FOR SCALE.          SETV 049
      CALL F01CAF(VCV, NPAR, NPAR, IFAULT)                                    SETV 050
      DO 30 I = 1, NVAR                                                       SETV 051
      DO 30 J = 1, I                                                          SETV 052
      IND = MINO(ISUB(I),ISUB(J))                                             SETV 053
      IND1 = MAXO(ISUB(I),ISUB(J))                                            SETV 054
      VCV(IND,IND1) = V(I,J)                                                  SETV 055
   30 CONTINUE                                                                SETV 056
      DO 40 J = 3, NPAR                                                       SETV 057
      DO 40 I = 1, J                                                          SETV 058
      TEMP = SIGMA * VCV(I,J)                                                 SETV 059
      IF (I .GE. 3) TEMP = SIGMA * TEMP                                       SETV 060
      VCV(I,J) = TEMP                                                         SETV 061
   40 CONTINUE                                                                SETV 062
C                                                                             SETV 063
C        FILL LOWER TRIANGLE OF VCV WITH CORRELATIONS.                        SETV 064
      DO 50 I = 2, NPAR                                                       SETV 065
      TEMP = VCV(I,I)                                                         SETV 066
      IND = I - 1                                                             SETV 067
      DO 50 J = 1, IND                                                        SETV 068
      IF (AMIN1(TEMP,VCV(J,J)) .LE. ZERO) GO TO 50                            SETV 069
      VCV(I,J) = VCV(J,I) / SQRT(TEMP*VCV(J,J))                               SETV 070
   50 CONTINUE                                                                SETV 071
C                                                                             SETV 072
      RETURN                                                                  SETV 073
      END                                                                     SETV 074
C*************************************************************************HESD 001
C        COMPUTES APPROXIMATE UPPER TRIANGLE OF HESSIAN BY DIFFERENCES.       HESD 002
C        NOTE THAT WITH IFLAG = 0, FUNCT WILL NOT SET A GRADIENT.             HESD 003
C        CALLED BY - VARIAB                                                   HESD 004
C        CALLS - FUNCT                                                        HESD 005
C*************************************************************************HESD 006
      SUBROUTINE HESDIF(PAR, NPAR, ISUB, H, SAVE1, SAVE2, NVAR, IW, LIW,HESD 007
     *W, LW)                                                                  HESD 008
C        ARGUMENTS                                                            HESD 009
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```
      INTEGER NPAR, NVAR, ISUB(NVAR), LIW, IW(LIW), LW                  HESD 010
      REAL PAR(NPAR), H(NVAR,NVAR), SAVE1(NVAR,NVAR), SAVE2(NVAR,NVAR), HESD 011
     *W(LW)                                                             HESD 012
C        LOCAL SCALARS                                                  HESD 013
      INTEGER ITER, IND, IND1, IND2, IND3                               HESD 014
      REAL PARI, PARJ, TEMP, TEMP1, STEP, DENOM, ZERO, TOL, TENM4,      HESD 015
     *STEP1, ONE, TWO, SQRT10, FOUR                                     HESD 016
      DATA ZERO, TOL, TENM4, STEP1, ONE, TWO, SQRT10, FOUR /0.0, 1.0E-6,HESD 017
     *1.0E-4, 3.162277660E-3, 1.0, 2.0, 3.162277660, 4.0/               HESD 018
C                                                                       HESD 019
C        START WITH STEPLENGTH 1.0E-3, REPEATEDLY DIVIDE BY             HESD 020
C        SQRT10. ITERATION STOPS WHEN DIFFERENCE BETWEEN SUCCESSIVE     HESD 021
C        HESSIANS LESS THAN 1.0E-6. IF NO SUCCESS IN 5 ITERATIONS,      HESD 022
C        USE RESULT WITH STEPLENGTH 1.0E-4.                             HESD 023
C        DIFFERENCE IS MAX. DIFFERENCE BETWEEN SUCCESSIVE ELEMENTS-     HESD 024
C          ABSOLUTE DIFFERENCE IF /LATEST ELEMENT/ .LT. 1,              HESD 025
C          RELATIVE DIFFERENCE IF /LATEST ELEMENT/ .GE. 1.              HESD 026
      ITER = 0                                                          HESD 027
      STEP = STEP1                                                      HESD 028
      DO 10 I = 1, NVAR                                                 HESD 029
      DO 10 J = I, NVAR                                                 HESD 030
   10 SAVE1(I,J) = ZERO                                                 HESD 031
C                                                                       HESD 032
C        STARTING POINT FOR ITERATION.                                  HESD 033
   20 ITER = ITER + 1                                                   HESD 034
      STEP = STEP / SQRT10                                              HESD 035
C                                                                       HESD 036
C        DIAGONAL ELEMENTS. THREE POINT DIFFERENCING.                   HESD 037
      DENOM = STEP * STEP                                               HESD 038
      DO 30 I = 1, NVAR                                                 HESD 039
      IND = ISUB(I)                                                     HESD 040
      PARI = PAR(IND)                                                   HESD 041
      PAR(IND) = PARI + STEP                                            HESD 042
      CALL FUNCT(0, NPAR, PAR, TEMP, PAR, IW, LIW, W, LW)               HESD 043
      PAR(IND) = PARI - STEP                                            HESD 044
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)              HESD 045
      TEMP = TEMP + TEMP1                                               HESD 046
      PAR(IND) = PARI                                                   HESD 047
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)              HESD 048
      H(I,I) = (TEMP - TWO*TEMP1) / DENOM                               HESD 049
   30 CONTINUE                                                          HESD 050
      IF (NVAR .EQ. 1) GO TO 50                                         HESD 051
C                                                                       HESD 052
C        OFF-DIAGONAL ELEMENTS IF REQUIRED. FOUR POINT DIFFERENCING.    HESD 053
      DENOM = FOUR * DENOM                                              HESD 054
      IND = NVAR - 1                                                    HESD 055
      DO 40 I = 1, IND                                                  HESD 056
      IND1 = I + 1                                                      HESD 057
      IND2 = ISUB(I)                                                    HESD 058
      PARI = PAR(IND2)                                                  HESD 059
      DO 40 J = IND1, NVAR                                              HESD 060
      IND3 = ISUB(J)                                                    HESD 061
      PARJ = PAR(IND3)                                                  HESD 062
      PAR(IND2) = PARI + STEP                                           HESD 063
      PAR(IND3) = PARJ + STEP                                           HESD 064
      CALL FUNCT(0, NPAR, PAR, TEMP, PAR, IW, LIW, W, LW)               HESD 065
      PAR(IND3) = PARJ - STEP                                           HESD 066
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)              HESD 067
      TEMP = TEMP - TEMP1                                               HESD 068
      PAR(IND2) = PARI - STEP                                           HESD 069
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      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)              HESD 070
      TEMP = TEMP + TEMP1                                               HESD 071
      PAR(IND3) = PARJ + STEP                                           HESD 072
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)              HESD 073
      H(I,J) = (TEMP - TEMP1) / DENOM                                   HESD 074
      PAR(IND2) = PARI                                                  HESD 075
      PAR(IND3) = PARJ                                                  HESD 076
   40 CONTINUE                                                          HESD 077
C                                                                       HESD 078
C        FIND DIFFERENCE, SAVE OLD HESSIAN IN SAVE1.                    HESD 079
   50 TEMP = ZERO                                                       HESD 080
      DO 60 I = 1, NVAR                                                 HESD 081
      DO 60 J = I, NVAR                                                 HESD 082
      PARI = H(I,J)                                                     HESD 083
      TEMP1 = ABS(PARI - SAVE1(I,J))                                    HESD 084
      PARJ = ABS(PARI)                                                  HESD 085
      IF (PARJ .GE. ONE) TEMP1 = TEMP1 / PARJ                           HESD 086
      TEMP = AMAX1(TEMP,TEMP1)                                          HESD 087
      SAVE1(I,J) = PARI                                                 HESD 088
   60 CONTINUE                                                          HESD 089
C                                                                       HESD 090
C        THIRD ITN, SAVE OLD HESSIAN IN SAVE2 (STEPLENGTH 1.0E-4).      HESD 091
      IF (ITER .NE. 3) GO TO 80                                         HESD 092
      DO 70 I = 1, NVAR                                                 HESD 093
      DO 70 J = I, NVAR                                                 HESD 094
   70 SAVE2(I,J) = H(I,J)                                               HESD 095
C                                                                       HESD 096
C        TEST STOPPING CRITERION FOR ITERATION.                         HESD 097
   80 IF (TEMP .LT. TOL) GO TO 100                                      HESD 098
      IF (ITER .LT. 5) GO TO 20                                         HESD 099
C                                                                       HESD 100
C        NO CONVERGENCE IN 5 ITNS - USE SAVE2, WITH STEP TENM4.         HESD 101
      STEP = TENM4                                                      HESD 102
      DO 90 I = 1, NVAR                                                 HESD 103
      DO 90 J = I, NVAR                                                 HESD 104
   90 H(I,J) = SAVE2(I,J)                                               HESD 105
C                                                                       HESD 106
C        EXIT, WRITE DETAILS (IND IS OUTPUT UNIT PASSED THROUGH IW),    HESD 107
C        AND SAVE THE NUMBER OF ITERATIONS REQUIRED.                    HESD 108
  100 IND = IW(4)                                                       HESD 109
      IW(1) = ITER                                                      HESD 110
      IF (IND .GT. 0) WRITE (IND,1000) ITER, STEP                       HESD 111
C                                                                       HESD 112
 1000 FORMAT (16HOHESSIAN DONE IN, I3, 6H ITNS,, 16H STEPSIZE USED =,   HESD 113
     *E11.3)                                                            HESD 114
C                                                                       HESD 115
      RETURN                                                            HESD 116
      END                                                               HESD 117
```

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This paper presents several families of algorithms for estimation of the parameters of the stable laws and the parameters of attracting stable laws. The paper also presents algorithms for estimation of the parameters of stable regression and stable autoregression models.

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