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Multidimensional Item Response Theory Estimation: A Computer Program

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MULTIDIMENSIONAL ITEM RESPONSE THEORY ESTIMATION:

A COMPUTER PROGRAM

(ONR REPORT 87-2)

VERSION 2.01

James E. Carlson

ABSTRACT

The MIRTE computer program, which provides estimates of item parameters and individuals' proficiencies (abilities) based on the multidimensional two-parameter logistic (M2PL) item response theory model, is described. The program uses a modified Newton-Raphson algorithm to iteratively estimate the parameters and proficiencies. The algorithm, use of the program, and some results based on simulated datasets are described.

Chapter 1

INTRODUCTION

The MIRTE computer program provides estimates of item parameters and individuals' proficiencies (abilities) for the model discussed by McKinley & Reckase (1983) and Reckase (1985). The method of estimation is a variation of the joint maximum likelihood procedure using a modified Newton-Raphson iterative technique. This report contains a brief overview of the model and the likelihood function, a description of the algorithm, a description of the input and output, and some data on performance of the program.

The Model and the Likelihood Function

The model underlying the program is the multidimensional extension of the two-parameter logistic (M2PL) model described by McKinley & Reckase (1983) and Reckase (1985):

$$\underline{P}_{ij} = \underline{P}(\underline{x}_{ij} = 1 | \mathbf{a}_i, \underline{d}_i, \theta_j) = \underline{c}_i + (1 - \underline{c}_i)\, e^{\underline{f}_{ij}}/(1 + e^{\underline{f}_{ij}}); \qquad (1)$$

$$\underline{f}_{ij} = \mathbf{a}_i'\,\theta_j + \underline{d}_i \quad (i = 1, 2, \ldots, \underline{K};\ j = 1, 2, \ldots, \underline{N}).$$

where:

$\underline{P}_{ij}$ = the probability of a correct response to item i by individual j;

$\underline{x}_{ij}$ = the response (1 = correct, 0 = incorrect) of individual j on item i;

$\mathbf{a}_i$ = a vector of $\underline{M}$ discrimination parameters for item i;

$\underline{d}_i$ = a parameter related to the difficulty of item i;

$\underline{c}_i$ = a fixed constant which may vary from item to item. It is the lower asymptote of the item response surface;

θ_j = a vector of $\underline{M}$ proficiency (ability) parameters for individual j;

$\underline{N}$ = the number of individuals;

K = the number of items;

M = the number of proficiency dimensions.

Note that c_i is a fixed constant rather than a parameter to be estimated. The user of the program must specify the values of c_i, which may be the same for each item. The model is sometimes referred to as the compensatory model because it allows high proficiency on one dimension to compensate for low proficiency on other dimensions in arriving at a correct response to a test item.

It is assumed that the response to each item, conditional on the proficiency vector, is independent of that to every other item. Hence, the likelihood of each K-element response vector $\mathbf{x}_j$ can be expressed as a product of probabilities:

$$\prod_{i=1}^{K} P_{ij}^{\,x_{ij}} Q_{ij}^{\,1-x_{ij}}$$

where: $Q_{ij} = 1 - P_{ij}$.

Assuming individuals respond to the items independently of one another, the likelihood of a set of N response vectors is also a product of probabilities:

$$L = \prod_{j=1}^{N} \prod_{i=1}^{K} P_{ij}^{\,x_{ij}} Q_{ij}^{\,1-x_{ij}} . \qquad (2)$$

Maximum Likelihood (ML) estimates of the parameters of the model are those values that maximize the likelihood function, L. Since it is easier to work with, and since its maximum occurs for the same values as L, we usually maximize the natural logarithm of L. Equivalently, we may define the ML estimates as the values:

$$\hat{a}_i,\ \hat{\underline{d}}_i,\ \hat{\theta}_j\ (i = 1, 2, \ldots, \underline{K};\ j = 1, 2, \ldots, \underline{N}), \tag{3}$$

that minimize the negative of the logarithm of $\underline{L}$:

$$\underline{F} = -\mathrm{Ln}(\underline{L}) \tag{4}$$

The Algorithm

The Basic Procedure

Finding estimates, (3), that minimize $\underline{F}$ in (4) involves finding the partial derivative of $\underline{F}$ with respect to each parameter in (1) and solving the equations resulting from setting the partial derivatives to zero. The matrix of second partial derivatives of $\underline{F}$ with respect to each pair of parameters must be positive definite to ensure a minimum is found. The equations to be solved are nonlinear and no direct solution is available, so an iterative procedure must be used to derive a series of successive approximations to the solutions. The iterative Newton-Raphson procedure for minimization consists of solving for a vector of unknowns, $\mathbf{w}$, by employing a set of initial estimates, $\hat{\mathbf{w}}_0$, and updating to achieve a better set of estimates:

$$\hat{\mathbf{w}}_1 = \hat{\mathbf{w}}_0 - \mathbf{H}_0^{-1}\mathbf{g}_0 \tag{5}$$

where $\mathbf{g}_0$ (the gradient) is the vector of first partial derivatives evaluated at the values in $\hat{\mathbf{w}}_0$, and $\mathbf{H}_0$ (the Hessian) the matrix of the second partial derivatives similarly evaluated. Letting $\underline{F}_0$ be the value of $\underline{F}$ evaluated at $\hat{w}_0$ and F_1 that evaluated at $\hat{w}_1$, the difference $F_0 - F_1$ (a positive number) is a measure of the improvement of $\hat{w}_1$ over $\hat{w}_0$. A second approximation, $\hat{w}_2$, is made by substituting $\hat{w}_1$ for $\hat{w}_0$, evaluating g_1 and H_1, and calculating $\hat{w}_2$ as in (5). The series of successive approximations is continued until the change in the evaluated value of F between successive stages falls below some small criterion value (converges). Expressions for the partial derivatives and second derivatives are provided in Appendix A. The joint maximum likelihood procedure as usually applied to item response theory (IRT) estimation problems (Wingersky, 1983; Hambleton & Swaminathan, 1985) consists of two parts: a set of iterations in which the current proficiency estimates are held constant (fixed) while iterations are performed on the item parameter estimates; and a set of iterations in which the current item parameter estimates are held fixed while iterations are performed on the individuals' proficiency estimates. In the algorithm used by the MIRTE program, a set of iterations is referred to as a phase. All phases consisting of iterations on proficiency estimates with fixed item parameters are identical. In estimating item parameters, however, there are two different types of iterations. In some phases the *a*-parameters are held fixed and iterations are performed only on the *d*-parameters. In other phases all item parameters are estimated. The MIRTE estimation algorithm combines several phases into a step and there are two types of steps between which it alternates. These will be referred to as "odd-numbered" and "even-numbered" steps. The following three sections describe the method of providing initial estimates (analogous to $\hat{w}_0$) in (5), and the nature of the phases in the even-numbered and the odd-numbered steps. This description assumes that both item parameters and subjects' proficiencies are to be estimated. The program also allows the estimation of item parameters holding proficiencies fixed in all phases, or proficiencies with item parameters fixed in all phases.

Initial Estimates

Before estimation begins, the program eliminates the data for any cases (persons) having perfect or zero number-right scores. These cases are identified in the output from the program. In order to commence iterations, it is necessary to have initial estimates of the proficiencies and the item parameters. The user must supply initial estimates of the discrimination parameters, a_i. These can be any number in the range

$$0 \leq \hat{\underline{a}}_{iko} \leq \hat{\underline{a}}_{max}$$

where $\hat{\underline{a}}_{iko}$ is the kth element of $\hat{a}_i$ and $\hat{\underline{a}}_{max}$ is a user definable maximum value for these discrimination parameters (the default value is 3.5). If all of the $\underline{a}_{iko}$ are started at zero for an item the algorithm will encounter problems because all the partial derivatives with respect to the $\underline{\theta}$'s will be evaluated to zero (see Appendix A). It is possible to set some $\underline{a}_{iko}$ to zero but it is probably better to choose nonzero starting values.

The initial difficulty parameters may, optionally, be supplied by the user of the program. It has been found, however, that the following formulas provide good initial $\underline{d}$-values and the program, by default, computes these "starting values":

$$\hat{\underline{d}}_{io} = \mathrm{Ln}\ \{\underline{z}_i/(1 - \underline{z}_i)\}$$

where

$$z_i = \prod_{j=1}^{N} x_{ij}/N$$

In order to avoid computational problems, the quantity in braces for these initial difficulty estimates is constrained to the open interval (0.0001, .9999). The $\hat{d}_{io}$ are also transformed to a mean of zero and standard deviation of 2 before commencing iterations. Initial values for the proficiency estimates are first computed as

$$\hat{\theta}^{*}_{jko} = \sum_{i=1}^{K} \hat{a}_{iko} x_{ij}$$

These values are then either orthonormalized using the Gram-Schmidt procedure or scaled to zero mean and unit variance. Orthonormalization is a user-selectable option and the default is to rescale to zero mean and unit variance.

As was mentioned above, the c_i are fixed constants rather than parameters to be estimated. The user of MIRTE must supply the values of these constants as input to the program. The c_i may be specified to be the same for all items and the common value may be specified as zero.

Odd Numbered Steps

For item parameter estimation phases within each odd-numbered step, the current estimates of the proficiencies are held fixed while iterations are performed on the d-parameter estimates. As mentioned above, all item parameters are held fixed in proficiency estimation phases. Hence an odd-numbered step proceeds as follows:

Phase 1: hold $\hat{a}_i$ and $\hat{\underline{d}}_i$ at current values; iterate on $\hat{\theta}_j$,

Phase 2: hold $\hat{a}_i$ and $\hat{\theta}_j$ at current values; iterate on $\hat{\underline{d}}_i$.

Additional phases are computed, with odd-numbered phases identical to phase 1 in form, and even-numbered phases identical to phase 2. Within each phase, iterations are performed independently on each individual (for proficiency estimation) or item (for item parameter estimation) because both items and individuals have likelihood equations (from setting the first derivatives to zero) that are independent of other individual's or item's equations.

Iterations proceed within each phase until either:

1. Convergence is reached; that is, all parameters being estimated change less than a user-specifiable criterion value for iterations (default = .05); or,
2. A user-specifiable maximum number of iterations is reached (default = 16).

Phases continue within each step until either:

1. $-\underline{u} \leq$ change in F between two successive phases $\leq \underline{u}$, where $\underline{u}$ is a user-definable constant (default value is 5.0); or,
2. change in F between two successive phases $< -\underline{u}$.

Even-numbered Steps

For item parameter estimation phases within each even-numbered step, the current estimates of the proficiencies are held fixed while iterations are performed on all the item parameter estimates. Iterations proceed on the item parameter estimates until convergence is reached or a maximum number of iterations has been carried out. The criteria are the same as for odd-numbered steps, as are the defaults (less than .05 change in all estimates or 16 iterations). Proficiency estimation phases, as is always the case, involve holding all item parameter estimates fixed. Phases continue to be computed as in the odd-numbered steps.

There is an option in the program to begin by estimating all item parameters, including the *a*-parameters, in step 1.

Convergence of Steps

Within each step, several phases are computed until a convergence criterion for steps is reached. This criterion is a specified amount of change in the computed value of F (the negative log likelihood function) between successive phases, as mentioned above. The criterion amount is user-selectable. The default is 5.0. As mentioned above, the likelihood function is evaluated initially (F_0) and at each phase (F_1, F_2, F_3, ...). At phase 1 the change is $F_0 - F_1$. The change in F between phases should always be a positive number. Occasionally a small negative value can occur. If a negative change of less than the criterion amount occurs, the program proceeds as usual. Occasionally a larger negative change may occur. This appears to be the result of attempting to use the program with too few items or too few cases (individuals), with the result that too many estimates are set to constrained extremes. Item response data generated from models other than the M2PL model have also resulted in negative changes in F, especially data from a three-parameter model. When the program detects a negative change (increase in F of more than the criterion) between phases, it stops computing additional phases in that step. Rather, it proceeds to the next step. If there are two consecutive negative changes the program stops executing and outputs results from the last step having a positive or zero change. At phase 2, the change is $\underline{F}_1 - \underline{F}_2$ at phase 3, $\underline{F}_3 - \underline{F}_2$, etc. If this value is lower than the criterion for two successive phases, the step is declared converged and the program proceeds to the next step.

Numbers of Steps and Phases

The number of steps and maximum number of phases to be performed can be specified by the user. The defaults are currently four steps and 60 phases. It should be noted that phases are numbered overall rather than within steps. Hence, the default is a total of 60 phases, not 60 phases per step. The number of phases is usually less than 25, but may be higher with larger datasets. Increasing the maximum allowed $\underline{a}$-parameter estimate will tend to increase the number of steps but may give a better solution (smaller value of $\underline{F}$).

The program continues until the maximum number of steps or phases is reached, or negative changes in $\underline{F}$ greater than the criterion occur for two consecutive phases. In general, it has been found that four steps are sufficient for overall convergence and rarely will using more than four provide a better solution.

Scaling and Constraining the Estimates

Because of an indeterminancy in the model, it is necessary to scale the estimates of the parameters. It is readily apparent in the expression for $\underline{f}_{ij}$ in (1) that multiplying each element of $\mathbf{a}_i$ by a constant, and multiplying the corresponding element of $\boldsymbol{\theta}_j$ by the reciprocal of that constant leaves the value unchanged. Hence an infinite number of sets of estimates can result in the same value of f_{ij}. In order to circumvent this indeterminancy, which is common to all IRT estimation algorithms, the proficiency estimates for each dimension are scaled to zero mean and unit variance after each step in which they are estimated. It is also necessary to rescale the item parameter estimates so that the f_{ij} and F remain constant.

If $\hat{\boldsymbol{\theta}}_j$ is rescaled to, say (where a bar over an estimate represents the mean estimate and S represents the standard deviation of the estimates),

$$\hat{\theta}^*_{jm} = \frac{\hat{\theta}_{jm} - \bar{\hat{\theta}}_m}{S_{\hat{\theta}_m}} \qquad (m = 1, 2, \ldots, M) \tag{6}$$

while $\hat{\mathbf{a}}_i$ is rescaled to

$$\hat{a}^*_{im} = S_{\hat{\theta}m}\, \hat{a}_{im} \qquad (m = 1, 2\ldots, M) \tag{7}$$

and d_i to

$$\hat{d}^*_i = \hat{d}_i + \hat{a}_{i1}\bar{\hat{\theta}}_1 + \hat{a}_{i2}\bar{\hat{\theta}}_2 + \ldots + \hat{a}_{iM}\bar{\hat{\theta}}_M \tag{8}$$

then it can be seen that

$$\sum_{m=1}^{M} \hat{a}^*_{im}\hat{\theta}^*_{jm} + \hat{d}^*_i = \sum_{m=1}^{M} \hat{a}_{im}\hat{\theta}_{jm} + \hat{d}_i$$

so that f_{ij} will remain the same after the rescaling. Hence (7) and (8) provide the formulas by which the discrimination and difficulty parameter estimates are rescaled after rescaling the proficiency estimates.

As is done in other IRT estimation algorithms such as LOGIST (Wingersky, Barton, & Lord, 1982), it is necessary to constrain the estimates at each stage in the MIRTE estimation program to prevent them from drifting to unreasonably large or small values. The user may specify maximum and minimum values of the proficiency estimates. The minimum (maximum) value used by the program for the difficulty estimates is the minimum (maximum) value for the theta estimates. As each of these parameters is re-estimated at each iteration, if it becomes higher (lower) than the limit, it is set to the limit. The program defaults are -4.5 and +4.5 for the theta estimates and hence also for the *d*-parameter estimates. Since negative discrimination parameters imply that a lower probability of getting an item correct is associated with higher proficiency, which would be counter to the IRT assumptions, the *a*-parameter estimates are constrained to a lower bound of zero. The actual lower bound is .01 to prevent all *a*-parameters becoming zero for an item, which would result in a totally nondiscriminating item. An upper bound can be specified by the user and the default value in the program is 3.5. Thus, if at any iteration a discrimination parameter estimate is zero or negative, it is set to .01, and if it exceeds the upper limit, it is set to that limit. Limits are set on all estimates before they are rescaled. Hence, the rescaled estimates for values set to limits may not equal the limits chosen by the user.

As estimates are rescaled after each phase in which proficiencies are estimated they are again compared to the upper and lower bounds and constrained to stay within these bounds. This constraint usually results in a slight change in the computed value of *F*. For the user's information *F* is output both before and after rescaling.

The program always indicates with the output of each estimate if it: a) failed to converge, b) was set to a limit, or, c) both failed to converge and was set to a limit.

Estimates of Standard Errors

Asymptotic variances and covariances of the estimated parameters can be estimated by taking the inverse of the matrix of second partial derivatives (used in the iterative estimation) evaluated at the last iteration. As pointed out by Hambleton and Swaminathan (1985), these estimates are approximations because the true values of the proficiencies are required to compute variances of the item parameter estimates and vice versa. The MIRTE program computes the square roots of the variances of the estimates to yield estimates of the standard errors of all of the parameters. It may be seen from (6) and (7) that the estimates of the standard errors of the $\underline{\theta}$s and $\underline{a}$s must be rescaled each time the parameter estimates are rescaled. This is done by the program.

Estimates of Multidimensional Item Parameters

When a final solution is attained, the multidimensional item parameters derived by Reckase (1985, 1986) are estimated and printed out. These parameters are:

1. Multidimensional Difficulty

Reckase (1985) defined this parameter for item i as

$$\underline{D}_i = - \underline{d}_i / \left(\sum_{m=1}^{\underline{M}} \underline{a}_{im}^2 \right)^{\frac{1}{2}}.$$

This parameter is the distance along a line perpendicular to the equiprobable contours of the item response surface from the origin of the space to the (1.0 + c_i)/2 contour. The line is at an angle of α_{ik} to the kth proficiency dimension where

$$\cos \alpha_{ik} = a_{ik} / \left(\sum_{m=1}^{M} a_{im}^2 \right)^{\frac{1}{2}} \tag{9}$$

2. Multidimensional Discrimination

Reckase (1986) defined this parameter for item i as

$$\text{MDISC} = \left(\sum_{m=1}^{M} a_{im}^2 \right)^{\frac{1}{2}}$$

It is related to the item characteristic curve on the multidimensional item response surface above the line defining D and a vector of angles, $\boldsymbol{\alpha}$. More specifically it is proportional to the slope of that curve at the point of steepest slope and is thus analogous to the unidimensional discrimination parameter.

In the MIRTE program we denote the multidimensional discrimination parameter as

$$\gamma_i = \left(\sum_{m=1}^{M} a_{im}^2 \right)^{\frac{1}{2}} = (\mathbf{a}_i{}'\mathbf{a}_i)^{\frac{1}{2}} \tag{10}$$

and the multidimensional difficulty parameter as

$$\beta_i = -d_i / \gamma_i \tag{11}$$

Denoting $\boldsymbol{\delta}_i$ as a vector of the cosines of the angles in (9)

$$\boldsymbol{\delta}_i = \begin{bmatrix} \cos \underline{\alpha}_{i1} \\ \cos \underline{\alpha}_{i2} \\ \vdots \\ \cos \underline{\alpha}_{iM} \end{bmatrix}$$

it may be seen from (9) that

$$\mathbf{a}_i = \underline{\gamma}_i \boldsymbol{\delta}_i \tag{12}$$

so that, using (11) and (12) we may write $\underline{f}_{ij}$ in (1) as

$$\underline{f}_{ij} = \underline{\gamma}_i (\boldsymbol{\delta}_i{}' \boldsymbol{\theta}_j - \underline{\beta}_i) \tag{13}$$

Noting that the inner product $\boldsymbol{\delta}_i{}' \boldsymbol{\theta}_j$ is a scalar we can replace it by, say, $\underline{\theta}^*_{ij}$ to write the exponent in model (1) as

$$\underline{f}_{ij} = \underline{\gamma}_i (\underline{\theta}^*_{ij} - \underline{\beta}_i) \tag{14}$$

This last expression is the exponent in representing the multidimensional parameters for item i according to the unidimensional item characteristic curve referred to above. It must be emphasized, however, that $\underline{\theta}^*_{ij}$ varies from item to item since the angles whose cosines are given is $\boldsymbol{\delta}_i$ vary. If they do not vary we have a truly unidimensional proficiency space.

The MIRTE computer program outputs estimates of $\underline{\gamma}_i$, $\underline{\beta}_i$, and the $\underline{\alpha}_{ki}$, computed using (9), (10), and (11) with estimates replacing the $\underline{a}_{ik}$ and $\underline{d}_i$.

Analysis of Residuals

For the final solution the program computes an estimate of $\underline{P}_{ij}$ by substituting estimates of $\mathbf{a}_i$, $\underline{d}_i$, and θ_j into (1). It then computes residuals, $\underline{r}_{ij} = \underline{x}_{ij} - \hat{\underline{P}}_{ij}$, for each individual on each item. The variance of the residuals for each item, and covariances between all pairs of items are also computed. The user may choose to have the values of these variances and covariances output. The covariances involving each item are ordered from highest to lowest before being output. Covariances between the residuals of each item and the estimated proficiencies on each dimension are also computed when this option is selected. The program always outputs a summary of the distribution of residual covariances.

Performance of the Program

The program was written in ANSI standard Fortran using the Ryan McFarland Fortran Compiler for the IBM PC and compatibles. Both interactive and batch versions have been created for these computers. A batch version has also been created and run on an IBM mainframe. All of the important computations are done in double precision.

In order to evalue the MIRTE program, a number of simulated datasets have been generated and analyzed. Simulated item parameters are generated for each item by:

1. Generating a pseudo-random angle, $\underline{\alpha}_1$, from a uniform distribution on the interval $(0, \pi/2)$;

2. Generating a pseudo-random multidimensional difficulty, β_i, from a normal distribution with mean zero and standard deviation 1.0;

3. Generating a pseudo-random multidimensional discrimination, γ_i, from a normal distribution with mean 1.7 and standard deviation .2; and

4. Computing $\mathbf{a}_i$ and d_i using (9), (10), and (11).

5. If nonzero values of c_i are specified they are incorporated into the generation process.

The simulated proficiencies are generated as pseudo-random variables from a bivariate normal distribution with specified correlation (varying from dataset to dataset) and means of zero and standard deviations of one. Finally, for each simulated subject on each simulated item, P_{ij} is computed from (1), and compared to a pseudo-random variable, R_{ij}, generated from a uniform distribution on the interval (0, 1). If $R_{ij} \le P_{ij}$ then x_{ij} is set to 1, otherwise it is set to zero. This results in an N by K matrix of data to be analyzed by MIRTE. In analyzing these datasets the starting values for the iterations on the a-parameters are generated using steps 1 through 4, above.

The program appears to be sensitive to the distribution of the discrimination parameters in the generated data. When data were generated with β having a standard deviation of .7, and γ having a mean of 1.2 and standard deviation of .2, the program did not converge and the estimates of a-parameters that were printed out did not correlate with the generating parameters. The proficiency and d-parameter estimates did not correlate as highly with the generating values as in other datasets but they were better than the a-parameter estimates.

To date, 16 datasets have been analyzed with constant c. Five of these had 2000 subjects and 60 items, one had 2000 subjects and 104 items, five had 500 subjects and 50 items, and five had 200 subjects and 30 items. Datasets were generated with correlations of 0, .3, .5, or .7 between the two proficiency dimensions. Means and standard deviations of estimates have been compared to those of the generating parameters, and correlations between the estimates and parameters have been computed. In general, the results, summarized in Table 1, are excellent for the large (*N* = 2000, *K* = 60 or 104) datasets, and quite good for smaller ones (*N* = 500, *K* = 50 and *N* = 200, *K* = 30). Correlations between the two estimated proficiency dimensions, however, tend to be smaller than the correlations between the generating proficiencies. The *d*-parameters are estimated very well with sample sizes as low as 500 and tests of 50 items, provided that the correlation between the generating proficiencies is .3 or less. *It is not recommended that datasets smaller than this be analyzed with MIRTE* even though good estimates of the *d*-parameters may be obtained.

One dataset of each size was generated from a model with a lower asymptote, *c*, of .2 and analyzed specifying all c_i to be zero. These datasets, as might be expected, exhibited difficulty in converging and resulted in very poor estimates of the *a*-parameters. The estimates of the *d*-parameters and proficiencies were, however, surprisingly good in the large datasets.

Two additional datasets having nonzero lower asymptotes for the item response surfaces were also examined, as shown in the bottom section of Table 1. One dataset had a constant *c*-parameter value of .15 for all items and the other had randomly generated (normal with mean .1, standard deviation .1) *c*-parameters for the 50 items. Results for these datasets were not quite as good as for the datasets having zero lower asymptotes as can be seen in the table.

The second datset was analyzed twice--once with the *c*-parameters fixed to the value used to generate the data for each item, and once with the *c*-parameter fixed to .1 for each item.

Results from analysis of one dataset consisting of 2000 simulated examinees and 60 simulated items are displayed in Tables 2 to 4. The dataset was analyzed twice with different randomly generated starting values for the *a*-parameters.

Table 2 shows the history of the *F* function during estimation steps and phases for one run. Note that two very small negative changes occurred.

TABLE 1

Correlational Results for Simulated Datasets

Description of Dataset				Correlations			
N	K	c	r_{θ_1,θ_2}	$\hat{\theta}_1,\hat{\theta}_2$	$\theta,\hat{\theta}$	$a,\hat{a}$	$d,\hat{d}$
Datasets fit with zero c-parameter							
2000	60	.0	.0	.014	(.915, .909)	(.978, .970)	.996
2000	60	.0	.0	.068	(.907, .925)	(.975, .976)	.999
Second Set of Starting Values					(.924, .908)	(.977, .975)	.999
2000	60	.0	.3	.256	(.916, .888)	(.980, .977)	.997
2000	60	.0	.5	.388	(.927, .908)	(.979, .960)	.997
2000	60	.2[1]	.0	.014	(.915, .909)	(.103, .007)	.934
2000	104	.0	.0	-.027	(.962, .952)	(.986, .984)	.998
500	50	.0	.0	-.025	(.907, .885)	(.928, .915)	.994
500	50	.0	.3	.109	(.936, .910)	(.903, .853)	.994
500	50	.0	.5	.180	(.913, .886)	(.878, .886)	.994
500	50	.0	.7	.054	(.879, .676)	(.786, .750)	.991
500	50	.2[1]	.0	.001	(.595, .362)	(.019,-.076)	.989
200	30	.0	.0	-.122	(.822, .811)	(.800, .741)	.978
200	30	.0	.3	-.338	(.719, .660)	(.734, .728)	.970
200	30	.0	.5	.052	(.801, .710)	(.609, .596)	.952
200	30	.0	.7	-.144	(.673, .646)	(.531, .466)	.966
200	30	.2	.0	-.546	(.619, .537)	(.506, .265)	.940
Datasets fit with nonzero c-parameter							
2000	60	.15	.0	-.204	(.846, .823)	(.897, .835)	.977
2000	50	{ }[2]	.0	-.219	(.855, .830)	(.960, .947)	.993
2000	50	{ }[3]	.0	-.236	(.855, .830)	(.958, .944)	.990

[1]MIRTE did not converge
[2]c-parameter varied in generation and fitting
[3]c-parameter varied in generation but set to .1 in fitting

TABLE 2

Dataset 1: 2000 Cases and 60 Items

History of Negative Log Likelihood Function

Step	Phase	-Ln(Like)	Change
0	0	54666.9	
1	1	52178.6	2488.31
1	2	51987.6	190.97
1	3	51838.6	148.98
1	4	51797.8	40.82
1	5	51794.9	2.94
1	6	51797.6	-2.79
2	1	50960.0	837.70
2	2	50781.9	178.05
2	3	50511.8	270.09
2	4	49862.9	648.93
2	5	48921.6	941.26
2	6	48035.1	886.56
2	7	47630.9	404.14
2	8	47462.4	168.56
2	9	47402.9	59.45
2	10	47378.3	24.60
2	11	47365.9	12.43
2	12	47358.7	7.21
3	1	47358.7	-.04
3	2	47358.6	.13
4	1	47353.1	5.51
4	2	47349.2	3.90

Note: If Two Successive Phases have Changes that are Within +/- the Phase Criterion (15.50) of zero, the Phase is Defined to be Converged

Execution Halted Because Of:

Maximum Number of Steps Reached

Tables 3 and 4 show descriptive statistics on the proficiency and item parameters, respectively, as well as statistics on the estimates, and the interrelations between parameters and their estimates. Note that in Table 3, for the second run, the first estimated theta dimension relates to the second true theta dimension and the second estimated to the first true. There is, of course, no way the program can differentiate one dimension from another in the order in which they are derived. This does not, however, present any problem for interpretation of results of the analysis of real data. The results in Table 3 show that the program does an excellent job of estimating the proficiency dimensions for this dataset.

Table 4 shows statistics for the item parameters and their estimates for the generated dataset for the two runs. The correlations among the various variables indicate high relationships between parameters and their estimates. Note that, consistent with the proficiency estimates, for the second run the $\underline{a}_1$ parameter estimates are related to the $\underline{a}_2$ parameters, and vice-versa. The table shows that the program also does an excellent job of estimating the item parameters for this dataset.

Although every attempt has been made to ensure that the program works correctly and outputs correct results, the complexity of the algorithm makes it impossible to guarantee that it will always work without error. Any user of MIRTE who finds an apparent error in the program is requested to report it to the author.

TABLE 3

Statistics on Generating Proficiencies & MIRTE Estimates

	Correlations						
		First Run		Second Run		Mean	St. Dev.
	$\underline{\theta}_2$	$\hat{\underline{\theta}}_{11}$	$\hat{\underline{\theta}}_{12}$	$\hat{\underline{\theta}}_{21}$	$\hat{\underline{\theta}}_{22}$		
$\underline{\theta}_1$	-.037	.907	.066	.033	.908	.001	1.001
$\underline{\theta}_2$		.069	.925	.924	.051	-.005	.999
$\hat{\underline{\theta}}_{11}$			.068	.033	1.000	.013	1.028
$\hat{\underline{\theta}}_{12}$				.999	.049	-.004	1.009
$\hat{\underline{\theta}}_{21}$					.014	-.004	1.009
$\hat{\underline{\theta}}_{22}$						.013	1.028

TABLE 4

Statistics on Generating Item Parameters & MIRTE Estimates

	Correlations									
			First Run			Second Run			Mean	St. Dev.
	$\underline{a}_2$	$\underline{d}$	$\hat{\underline{a}}_{11}$	$\hat{\underline{a}}_{12}$	$\hat{\underline{d}}_1$	$\hat{\underline{a}}_{21}$	$\hat{\underline{a}}_{22}$	$\hat{\underline{d}}_2$		
$\underline{a}_1$	-.828	.092	.975	-.856	.101	-.850	.979	.101	1.074	.481
$\underline{a}_2$		-.161	-.861	.976	-.173	.975	-.847	-.172	1.141	.505
$\underline{d}$			.087	-.183	.999	-.194	.078	.999	.070	1.704
$\hat{\underline{a}}_{11}$				-.876	.095	-.869	.999	.095	1.118	.648
$\hat{\underline{a}}_{12}$					-.197	1.000	-.864	-.197	1.194	.660
$\hat{\underline{d}}_1$						-.209	.087	1.000	.078	1.789
$\hat{\underline{a}}_{21}$							-.858	-.208	1.215	.652
$\hat{\underline{a}}_{22}$								.087	1.155	.624
$\hat{\underline{d}}_2$									.069	1.784

Chapter 2

INPUT TO THE PROGRAM

The dataset to be analyzed is described to MIRTE in a series of records described below. In the description, records containing the numeric input (and formats) for starting values, item responses, etc., are referred to as "Data Records" in order to distinguish them from the records that describe the problem run to the program. The latter are referred to as "Input Description Records."

In general the Input Description Records can be in any order. Most of these records are optional. Each begins with a unique Record Name, which must begin in column 1. The ITEMS Record which conveys to the program the number of items is required and must precede any Data Records. An INPUT DATA Record is also required and must be the last Input Description Record. An ITEM PARAMETERS Record is also required.

In order to allow the user flexibility in labeling a problem run, any number of title records may be included among the Input Description Records. The program assumes that any record that it does not recognize as a Data Record or an Input Description Record is a title record. The exact contents of these records are printed near the beginning of the output. As a result, misspelling the name of an Input Description Record will cause that record to be treated as a title record.

Each Input Description Record (except title records) must begin with its Record Name which must be capitalized and begin in column 1. These records contain keywords after their names. Most of the keywords are optional and they may be placed in any order on the record. The only required keyword is that specifying the number of items (on the ITEMS Record). Keywords must be capitalized and may be separated either by blanks or commas. Other punctuation on the Input Description Records is ignored by the program so the user may include additional punctuation as separators if he/she wishes to do so. The author has found it convenient to separate Record Names from keywords with colons, and to separate keywords from each other with both a comma and a blank. The reason for this is that several keywords consist of two words which must be separated by blanks. An example of input to the program is provided in Figure 1 described later.

Input Description Records

Each record is described below. Item Records and Keywords with asterisks (*) are required. All others are optional. All words and letters must be capitalized.

Name of Record	Keywords	Comments
*ITEMS	*N=#	- Required: There is no default. - # is the number of items. - No blank spaces are allowed within this keyword (Example N=35).
	FIXED	- Included when only proficiencies are to be estimated from fixed input parameters.
	PRINT STEPS	- If included, item parameter estimates are printed after each step of the estimation process. - If it is not included only the starting values and final estimates are printed. - Must contain exactly one space between PRINT and STEPS.

Name of Record	Keywords	Comments
ITEMS (continued from previous page)	PRINT FINAL	- Necessary only when FIXED is specified and the user wants the item parameter estimates printed after the final step. - Requires exactly one space between PRINT and FINAL.
	FILE=#	- Used when the user wishes to save the final parameter estimates in a file. - Each record of the file contains the *M* *a*-parameter estimates, followed by the *d*-parameter estimate, from one item. - The format is (1X,10F7.3). - Output defaults to unit number 9 unless the =# Keyword is used (=# is optional). - # is the optional unit number, necessary if 9 not to be used. - No blank spaces allowed within the keyword (Example FILE=11).
SUBJECTS	N=#	- Not required: By default MIRTE counts the number of subjects. - # is the number of subjects. - No blank spaces are allowed within this keyword (Example N=2500).
	FIXED	- Included when only item parameters are to be estimated from fixed proficiencies. - *A PROFICIENCIES Record is required when this keyword is specified*.
	PRINT STEPS	- If included, proficiency estimates are printed after each step of the estimation process (Warning! *This can generate a great deal of output*). - No proficiency estimates are printed by default. - Requires exactly one space between PRINT and STEPS.
	PRINT FINAL	- If included, proficiency estimates are printed after the final step. This will generate *N* lines of output. - No proficiency estimates are printed by default. - Requires exactly one space between PRINT and FINAL.

Name of Record	Keywords	Comments
SUBJECTS (continued from previous page)	FILE=#	- Used when the user wishes to save the final proficiency estimates in a file. - Each record of the file contains the M proficiency estimates for one subject. - The format is (1X,11F7.3). - Output defaults to Unit Number 8 unless the =# Keyword is used (=# is optional). - # is the optional Unit Number, necessary if 8 not to be used. - No blank spaces allowed within the keyword (Example FILE=1).
RESIDUALS	FILE=#	- If this keyword is specified the residuals are output to a file. - Output defaults to Unit Number 11 unless the =# Keyword is used (=# is optional). - # is the optional unit number, necessary if 11 not to be used. - The format is (1X,11F7.3).
	FULL	- If this keyword is specified the residual variances and covariances for each item are printed. - The FULL residual analysis is not printed in the output unless this keyword is specified. A summary is always printed.
*INPUT DATA		- Exactly one space required between INPUT and DATA. - Must be followed by the item response data records unless the data are in a file to be connected at run time. In that case a UNIT= Keyword must be specified. - Item response data must consist of ones (correct) and zeros (incorrect). One or more records per subject, controlled by the format. - To save space, item response data are stored by MIRTE as CHARACTER*1 data. Hence the format must contain A1-fields, e.g., (40A1).

Name of Record	Keywords	Comments
INPUT DATA (continued from previous page)		- If the user supplies a format it must be the first data record in the input response data. Hence if those data follow the INPUT DATA Record in the primary input stream, the format must be immediately after that Record. If the data are in a file separate from the Input Description Records, the format must also be in that separate file (and must be the first record of that file).
	UNIT=#	- Used to specify the Unit Number of the device containing the item response data records, if those records are not in the main input stream along with the INPUT DATA and other Input Description records. - No spaces allowed (e.g., UNIT=24).
	DEFAULT FORMAT	- If this keyword is specified there may be no format record for the item response data. These data will then be read by the format (100A1). - Requires exactly one space between DEFAULT and FORMAT.
STEPS	MAXNUM=#	- Used to specify the maximum number of steps if the default of 4 is not to be used. - No spaces allowed (e.g., MAXNUM=6).
	CRI=#	- Used to specify the amount of change in F defining convergence of phases. Enter as a whole number or with a decimal fraction. - The default is 5. - No spaces allowed (e.g., CRI=35).
PHASES	MAXIT=#	- Used to specify the maximum allowed number of iterations within each stage (for both item parameter estimation and proficiency estimation iterations) if the default of 16 is not to be used. - No spaces allowed (e.g., MAXIT=10).
	CRI=.#	- Used to specify the convergence criterion for all iterations within each stage if the default of .05 is not to be used. - Must be entered with a decimal point. - No spaces allowed (e.g., CRI=.01).

Name of Record	Keywords	Comments
PHASES (continued from previous page)	CRI=.# (cont.)	- When an item parameter estimate or proficiency estimate changes by less than CRI in any iteration, no more iterations are performed on that estimate during that phase. The program indicates how many estimates met this criterion for each phase.
	MAXNUM=#	- Used to specify maximum number of phases if the default of 60 is not to be used. - No spaces allowed (e.g., MAXNUM=40).
LIMITS	TMIN=#	- Used to specify the minimum value of each proficiency estimate if the default of -4.5 is not to be used. - No spaces allowed (e.g. TMIN=-4).
	TMAX=#	- Used to specify the maximum value of each proficiency estimate if the default of 4.5 is not to be used. - Generally TMAX should equal -TMIN but it does not have to do so. - No spaces allowed (e.g., TMAX=3.75).
	AMAX=#	- Used to specify the maximum value of each a-parameter estimate if the default of 3.5 is not to be used. - No spaces allowed (e.g., AMAX=4.5). - NB: The user cannot specify a minimum value of the a-parameter estimates. This value is set by the program to .01 as discussed above.
	STARTA	- Used to instruct the program to begin by estimating item parameters including the <u>a</u>-parameter at step 1.
*ITEM PARAMETERS		- <u>Required</u> This record specifies the nature of input item parameters or estimates. - If the FIXED Keyword is used on the ITEMS Record the fixed values of the item parameters are input. Otherwise starting values for iterations are input. - If the FIXED keyword is not specified on the ITEMS record, no <u>d</u>-parameter starting values are input unless the SVDIF keyword is specified. - If the CPARM VARIES keyword is specified, the <u>c</u>-values are input with the starting values of the item parameters.

Name of Record	Keywords	Comments
*ITEM PARAMETERS (continued from previous page)		- If the UNIT=# keyword is used, # specifies the unit number by which the file containing parameters or starting values is accessed. If no unit number is specified, these values are on records following the ITEM PARAMETERS record. - The starting values (or parameters) for each item are input from a separate record, the M a-parameter values first, followed by the d-parameter value, and the c-value when it varies from item to item. If the FREE FORMAT keyword is not specified, a record containing a format statement must preceed the record for the first item parameter values. - Must contain exactly one space between ITEM and PARAMETERS.
	UNIT=#	- Used to specify the unit number of the device containing the item parameters data records (including the format record if one is used), if those records are not in the main input stream along with the ITEM PARAMETERS Record and the other Input Description Records. - No spaces allowed (e.g., UNIT=21).
	FREE FORMAT	- Used to specify that free format input is to be used for the item parameter data records. When free format is used those data records must have blanks or commas between the different parameters or starting values.
	SVDIF	- Used to specify that starting values are to be input for the difficulty parameters. By default the program will compute starting values.
	CPARM VARIES	- Used to specify that the c-constant varies from item to item. When this keyword is specified, the c-values for each item are input along with the initial a-parameters or estimates, and initial d-parameters or estimates when they are input. The order of input is as, ds, cs. - Exactly one space between CPARM and VARIES.

Name of Record	Keywords	Comments
*ITEM PARAMETERS (continued from previous page)	CPARM=#	- Used to specify the common value of the c-constant when it does not vary from item to item. The default value is zero.
PROFICIENCIES		- Used when FIXED is specified on the SUBJECTS Record. This record is ignored otherwise.
	UNIT=#	- Similar to that specified above for the ITEM PARAMETERS Record.
	FREE FORMAT	- Similar to that specified above for the ITEM PARAMETERS Record.
	SVTHET	- Used to specify that start values are to be input for the proficiency estimates. By default the program will compute its own starting values. Not necessary when the FIXED Keyword is used on the SUBJECTS Record.
	ORTHO	- Used to specify that the starting values for the proficiencies are to be orthornormalized before estimation begins. Should not be used when the FIXED Keyword is used on the SUBJECTS Record.
DIMENSIONS		- Only required if the number of dimensions is not 2.
	N=#	- Specified the number of dimensions which defaults to 2 if this keyword is not specified. - Must contain no spaces (e.g. N=3).

Example Input

Figure 1 shows an example input for a run of the MIRTE program. The first two lines (records) contain no Input Record Names and hence are title records for labeling the output. The DIMENSIONS Record specifies a two-dimensional solution. There are 15 items according to the ITEMS Record, and item parameter estimates are to be saved in a file connected, by default, via Unit 9. The proficiency estimates, are specified on the SUBJECTS Record to be saved in a file connected by default via Unit 8. The final proficiency estimates are also to be printed in the output from MIRTE. The maximum number of allowed steps is specified as 4 on the STEPS Record and the convergence criterion for steps is a change in the minimization function, $\underline{F}$, of 5.5 or less in two consecutive phases. According to the PHASES Record the maximum total number of phases is 40 and the maximum number of iteration per phase is 16. The criteria for convergence of estimates is a .05 change between two consecutive iterations. The maximum allowed $\underline{a}$-parameter estimate is specified on the LIMITS Record as 4.5. According to the RESIDUALS Record, residuals will be stored in a file connected, by default, to unit 11. A full Residual Analysis will also be printed out. Although there is a PROFICIENCIES Record in the input, it includes no keywords and hence is ignored by the program. Start value data records follow the ITEM PARAMETERS Record and they are to be read in free format from Unit Number 5. Each record contains the initial estimates of a_1, and a_2 for an item. The item response data records are to be input with the Input Description Records because UNIT Number 5 is specified. The data, in the form of 1s and 0s, complete the input file.

```
  Small Dataset, NS=50, NI=15
  For Debugging Purposes
DIMENSIONS: N=2
ITEMS: N=15, FILE
SUBJECTS: FILE, PRINT FINAL
STEPS: MAXNUM=4, CRI=5.5
PHASES: MAXNUM=40, MAXIT=16, CRI=.05
LIMITS: AMAX=4.5
RESIDUALS: FILE, FULL
PROFICIENCIES:
ITEM PARAMETERS: UNIT=5, FREE FORMAT
   0.688  1.399
   1.924  0.404
   1.671  0.338
   1.714  0.906
   0.804  1.537
   0.539  1.678
   0.885  1.458
   0.048  1.605
   1.246  0.458
   1.684  0.836
   1.297  1.518
   1.676  1.086
   1.406  0.602
   1.730  0.752
   1.418  0.000
INPUT DATA: UNIT=5, DEFAULT FORMAT
110111100111101
010111101011001
110011001001001
110111000001001
110111111001100
110001001100001
100111101001000
110111001101000
110111011101001
010011001000001
000101001101001
111110000000000
110111101001001
010000000011000
111111111111000
000111101000000
110111001111001
010011000100001
110111000110001
110111001101001
```

Figure 1. Example-Input (continued next page)

```
110111011111001
010000000000000
110110101001001
110111101111001
110111001111011
010100000100001
000111001011001
110111001110001
110111011110001
110000101111000
010011101101001
111011001101001
110111111011001
111111111111101
111111111001101
110101000001001
110011001101001
010010000001000
110111001110001
010111001011001
010010000000000
110010111001001
010001000100000
110001000110001
110101000100001
010101000110001
000001000001001
100111001110001
110100111111001
110100101011001
```

Figure 1. (continued)

Chapter 3

EXAMPLE OUTPUT

The output generated by the input displayed in Figure 1 are provided in Appendix B. These results are from a run on an IBM PC AT and some results will differ slightly from those from runs on a mainframe computer.

Page B2 of Appendix B is the title page which includes, at the bottom, all lines from the input file that are not recognized by the program as being either Input Description Records or Data Records. These should be records intended by the user to be titles for the output. Note, however, that any Input Description record whose name is misspelled will be listed here and not processed by the program.

The third page of the appendix lists the parameters of the job, including defaults as well as those specified by the user. In the section on page B4 labeled "Initial Item Parameter Estimates," the estimated values of _d_ were computed by the program using the method described in Chapter 1. The estimated values of the _a_-parameters are those input by the user (the same as those in Figure 1). If the option to vary the _c_-parameter over items is used the values of _c_ will also be printed here. The fourth page also shows the number of individuals who selected the correct answer to each item. There is also an indication of the number, if any, of subjects who received either zero or perfect scores. There were no such subjects in the example data, but when there are their data are not included in any computations. If the option to print proficiencies is selected by the user these subjects are denoted in the output file as having zero or perfect scores. Finally, the initial value of the negative of the log likelihood (_F_) is printed.

Pages B5 through B11 show the output provided for each step and each phase within each step. The user may also have estimates output at each step but this considerably increases the size of the printout. Page B12 contains the final item parameter estimates and the estimates of their standard errors. Page B13 shows the multidimensional item parameter estimates. The final proficiency estimates and their standard errors are displayed on pages B14 and B15 and the latter also shows the correlation between the estimated proficiency (theta) dimensions.

Pages B16 through B20 illustrate the form in which the residual variances and covariances are printed out when the "FULL" keyword appears on the "RESIDUAL" Input Description record. The residual variance for each item and the residual covariances with the estimated proficiencies (thetas) are printed first. These are followed by the values of the residual covariances with each of the other items, ordered in descending order. The latter have been found useful in detecting items that violate the local independence assumption underlying all IRT models. When items that violate this assumption have been generated and analyzed with a set of independent items the covariances between the dependent items have tended to be two to four times larger than those between independent items.

Page B21 contains a frequency distribution of the between-item residual covariances. This table is always printed, even when "FULL" is not specified on the RESIDUAL Record. <u>Note that the ranges are wider in the second half than the first half of this table</u>. The final page of the output shows the history of the negative log likelihood function over all the steps and phases, and the reason that the program stopped when it did. In the example it stopped because the maximum specified number of steps was reached. Note that there were two phases in which the changes in $\underline{F}$ were actually negative. Since the magnitude of none of these changes exceeded the convergence criterion of 5.5 (also printed on this page) the phases at which they occurred were declared converged.

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Appendix A

Partial Derivatives of the Negative Log Likelihood Function

Appendix A

Partial Derivatives of the Negative Log Likelihood Function

First Partial Derivatives

$$\frac{\partial F}{\partial \theta_{jm}} = \sum_{i=1}^{K} \frac{(P_{ij} - c_i)(P_{ij} - x_{ij})\, a_{im}}{(1 - c_i)P_{ij}}$$

$$(j = 1, 2, \ldots, N;\ m = 1, 2, \ldots, M)$$

$$\frac{\partial F}{\partial d_i} = \sum_{j=1}^{N} \frac{(P_{ij} - c_i)(P_{ij} - x_{ij})}{(1 - c_i)P_{ij}}$$

$$(i = 1, 2, \ldots, K)$$

$$\frac{\partial F}{\partial a_{im}} = \sum_{j=1}^{N} \frac{(P_{ij} - c_i)(P_{ij} - x_{ij})\theta_{jm}}{(1 - c_i)P_{ij}}$$

$$(i = 1, 2, \ldots, K;\ m = 1, 2, \ldots, M)$$

Second Partial Derivatives

$$\frac{\partial^2 F}{\partial \theta_{jm}^2} = \sum_{i=1}^{K} \frac{(P_{ij}^2 - c_i x_{ij})(P_{cj} - c_i)Q_{ij} a_{im}}{(1 - c_i{}^2 P_{ij}^2}$$

$$(j = 1, 2, \ldots, N;\ m = 1, 2, \ldots, M)$$

$$\frac{\partial^2 F}{\partial\theta_{jm}\partial\theta_{jn}} = \sum_{i=1}^{K} \frac{(P^2_{ij} - c_i x_{ij})(P_{ij} - c_i)Q_{ij}a_{im}a_{in}}{(1 - c_i)P^2_{ij}}$$

$(j = 1, 2, \ldots, N;\ m, n = 1, 2, \ldots M;\ m \neq n)$

$$\frac{\partial^2 F}{\partial d_i^2} = \frac{1}{(1 - c_i)^2} \sum_{j=1}^{N} \frac{(P^2_{ij} - c_i x_{ij})(P_{ij} - c_i)Q_{ij}}{P^2_{ij}}$$

$(i = 1, 2, \ldots, K)$

$$\frac{\partial^2 F}{\partial d_i \partial a_{im}} = \frac{1}{(1 - c_i)^2} \sum_{j=1}^{N} \frac{(P^2_{ij} - c_i x_{ij})(P_{ij} - c_i)Q_{ij}\theta_{jm}}{P^2_{ij}}$$

$(i = 1, 2, \ldots, K;\ m = 1, 2, \ldots, M)$

$$\frac{\partial^2 F}{\partial a_{im}^2} = \frac{1}{(1 - c_i)^2} \sum_{j=1}^{N} \frac{(P^2_{ij} - c_i x_{ij})(P_{ij} - c_i)Q_{ij}\theta^2_{jm}}{P^2_{ij}}$$

$(i = 1, 2, \ldots, K;\ m = 1, 2, \ldots, M)$

$$\frac{\partial^2 F}{\partial a_{im}\partial a_{in}} = \frac{1}{(1 - c_i)^2} \sum_{j=1}^{K} \frac{(P^2_{ij} - c_i x_{ij})(P_{ij} - c_i)Q_{ij}\theta_{jm}\theta_{jn}}{P^2_{ij}}$$

$(i = 1, 2, \ldots, K;\ m, n = 1, 2, \ldots M;\ m \neq n)$

Appendix B

Example Output

B2

```
MM    MM
MMM  MMM
MM M MM
MM    MM
MM    MM   U  L  T  I  D  I  M  E  N  S  I  O  N  A  L


          IIIIII
            II
            II
            II
          IIIIII   T  E  M


                    RRRRRR
                    RR    RR
                    RRRRRR
                    RR  RR
                    RR   RR   E  S  P  O  N  S  E


                             TTTTTTTT
                                TT
                                TT
                                TT
                                TT    H  E  O  R  Y
```

```
Two-parameter Compensatory Model          EEEEEE
                                          EE
Copyright (c)  James E. Carlson           EEEE
                                          EE
ACT, 1988,  All Rights Reserved.          EEEEEE S  T  I  M  A  T  I  O  N

Version 2.01
```

^^

Small Dataset, NS=50, NI=15

For Debugging Purposes

```
Number of Subjects:     50
Number of Items:     15
Number of Dimensions:      2
Maximum Number of Steps:      4
Convergence Criterion for Iterations:  0.050000
Maximum Number of Iterations:    16
Convergence Criterion for Steps:       5.50


Item Difficulty Estimates Constrained Not Less Than:    -4.500
     and Not Greater Than:    4.500
Person Proficiency (Theta) Estimates Constrained Not Less Than:    -4.500
   and Not Greater Than:    4.500
Item Discrimination Estimates Constrained Not Less Than:    0.010
   and Not Greater Than:    4.500
Common c-parameter of ZERO in the Model
Discrimination Start Values input from FILE #  1

Item Parameter Estimates Output to FILE #  9

Proficiency Estimates Output to FILE #  8

Residuals Output to FILE # 11

Final Proficiency Estimates to be Output

Full Residual Analysis to be Output

Both Item Parameters and Proficiencies (Thetas) will be Estimated
```

Initial Item Parameter Estimates

Item	d	a1	a2
1	1.101	0.688	1.399
2	2.605	1.924	0.404
3	-2.481	1.671	0.338
4	1.101	1.714	0.906
5	1.333	0.804	1.537
6	1.723	0.539	1.678
7	-0.619	0.885	1.458
8	-1.497	0.048	1.605
9	1.101	1.246	0.458
10	0.479	1.684	0.836
11	-0.107	1.297	1.518
12	0.991	1.676	1.086
13	-2.779	1.406	0.602
14	-4.500m	1.730	0.752
15	1.586	1.418	0.000

Number of Subjects = 50

Number Correct Scores for Items:

Items :	Scores									
1 - 10 :	34	44	5	34	36	39	17	10	34	28
11 - 15 :	22	33	4	1	38					

Initial Negative Log Likelihood: 0.32658081D+03

```
================================================================================

                         START OF STEP #    1

  Estimating Thetas and Difficulties with Fixed Discriminations

================================================================================

********************************************************************************

               Start of Phase #    1

 Theta Estimation: Convergence reached for   49 Cases in  16 Iteration(s)

 NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =     1

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

               Last Value of Negative Log Likelihood:  0.32658081D+03
               New Value of Negative Log Likelihood:   0.28774700D+03
                                         Difference:  0.38833807D+02

                    -Ln(Likelihood) after Rescaling:      0.28787050D+03

                    Phase Not Converged by Criterion of: +/-    5.5

 Step Not Converged: Convergence for  0 Successive Phase(s)

********************************************************************************

               Start of Phase #   2

 Item Estimation: Convergence reached for   14 items in  16 Iteration(s)

 NUMBER OF a-PARAMETER ESTIMATES SET TO MIN. OR MAX. =    1
 NUMBER OF d-PARAMETER ESTIMATES SET TO MIN. OR MAX =    1

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

               Last Value of Negative Log Likelihood:  0.28787050D+03
               New Value of Negative Log Likelihood:   0.28874275D+03
                                         Difference: -0.87225191D+00

                    Phase Converged by Criterion of: +/-    5.5

 Step Not Converged: Convergence for  1 Successive Phase(s)
```

```
********************************************************************************

              Start of Phase #   3

 Theta Estimation: Convergence reached for   49 Cases in  16 Iteration(s)

 NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =    1

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

              Last Value of Negative Log Likelihood:  0.28874275D+03
              New Value of Negative Log Likelihood:   0.28755214D+03
                                        Difference:  0.11906109D+01

                   -Ln(Likelihood) after Rescaling:       0.28764353D+03

                   Phase Converged by Criterion of: +/-    5.5

 Step Converged: Two Successive Phases Converged

================================================================================

                                  START OF STEP #   2

  Estimating Thetas and all Item Parameters

================================================================================


********************************************************************************

              Start of Phase #   1

 Item Estimation: Convergence reached for   14 items in  16 Iteration(s)

 NUMBER OF a-PARAMETER ESTIMATES SET TO MIN. OR MAX. =   1
 NUMBER OF d-PARAMETER ESTIMATES SET TO MIN. OR MAX =   1

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

              Last Value of Negative Log Likelihood:  0.28764353D+03
              New Value of Negative Log Likelihood:   0.26551269D+03
                                        Difference:  0.22130835D+02

                   Phase Not Converged by Criterion of: +/-    5.5

 Step Not Converged: Convergence for  0 Successive Phase(s)

********************************************************************************
```

```
*******************************************************************************

              Start of Phase #   2

 Theta Estimation: Convergence reached for   48 Cases in  16 Iteration(s)

 NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =    2

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

              Last Value of Negative Log Likelihood:  0.26551269D+03
              New Value of Negative Log Likelihood:   0.24543282D+03
                                         Difference:  0.20079865D+02

                   -Ln(Likelihood) after Rescaling:       0.24590862D+03

                   Phase Not Converged by Criterion of: +/-    5.5

 Step Not Converged: Convergence for  0 Successive Phase(s)


*******************************************************************************

              Start of Phase #   3

 Item Estimation: Convergence reached for   11 items in  16 Iteration(s)

 NUMBER OF a-PARAMETER ESTIMATES SET TO MIN. OR MAX. =   4
 NUMBER OF d-PARAMETER ESTIMATES SET TO MIN. OR MAX =   1

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

              Last Value of Negative Log Likelihood:  0.24590862D+03
              New Value of Negative Log Likelihood:   0.23257787D+03
                                         Difference:  0.13330753D+02

                   Phase Not Converged by Criterion of: +/-    5.5

 Step Not Converged: Convergence for  0 Successive Phase(s)
```

```
*******************************************************************************

            Start of Phase #   4

Theta Estimation: Convergence reached for   48 Cases in  16 Iteration(s)

NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =    2

MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

            Last Value of Negative Log Likelihood:  0.23257787D+03
            New Value of Negative Log Likelihood:   0.22096582D+03
                                      Difference:   0.11612052D+02

                -Ln(Likelihood) after Rescaling:       0.22386138D+03

                Phase Not Converged by Criterion of: +/-    5.5

Step Not Converged: Convergence for  0 Successive Phase(s)


*******************************************************************************

            Start of Phase #   5

Item Estimation: Convergence reached for    8 items in  16 Iteration(s)

NUMBER OF a-PARAMETER ESTIMATES SET TO MIN. OR MAX. =   7
NUMBER OF d-PARAMETER ESTIMATES SET TO MIN. OR MAX =   2

MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

            Last Value of Negative Log Likelihood:  0.22386138D+03
            New Value of Negative Log Likelihood:   0.22014558D+03
                                      Difference:   0.37157937D+01

                Phase Converged by Criterion of: +/-    5.5

Step Not Converged: Convergence for  1 Successive Phase(s)
```

```
********************************************************************************

               Start of Phase #    6

 Theta Estimation: Convergence reached for   48 Cases in  16 Iteration(s)

 NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =     2

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

               Last Value of Negative Log Likelihood:  0.22014558D+03
               New Value of Negative Log Likelihood:   0.21559717D+03
                                           Difference:  0.45484117D+01

                    -Ln(Likelihood) after Rescaling:        0.21762704D+03

                    Phase Converged by Criterion of: +/-     5.5

 Step Converged: Two Successive Phases Converged

================================================================================

                                  START OF STEP #    3

  Estimating Thetas and Difficulties with Fixed Discriminations

================================================================================


********************************************************************************

               Start of Phase #    1

 Item Estimation: Convergence reached for   12 items in  16 Iteration(s)

 NUMBER OF a-PARAMETER ESTIMATES SET TO MIN. OR MAX. =    7
 NUMBER OF d-PARAMETER ESTIMATES SET TO MIN. OR MAX =    3

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

               Last Value of Negative Log Likelihood:  0.21762704D+03
               New Value of Negative Log Likelihood:   0.22046897D+03
                                           Difference: -0.28419365D+01

                    Phase Converged by Criterion of: +/-     5.5

 Step Not Converged: Convergence for  1 Successive Phase(s)
```

```
*******************************************************************************

            Start of Phase #   2

 Theta Estimation: Convergence reached for   48 Cases in  16 Iteration(s)

 NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =    2

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

            Last Value of Negative Log Likelihood:  0.22046897D+03
            New Value of Negative Log Likelihood:   0.21770493D+03
                                     Difference:  0.27640464D+01

                 -Ln(Likelihood) after Rescaling:      0.21936595D+03

                 Phase Converged by Criterion of: +/-    5.5

 Step Converged: Two Successive Phases Converged

===============================================================================

                              START OF STEP #   4

  Estimating Thetas and all Item Parameters

===============================================================================


*******************************************************************************

            Start of Phase #   1

 Item Estimation: Convergence reached for    6 items in  16 Iteration(s)

 NUMBER OF a-PARAMETER ESTIMATES SET TO MIN. OR MAX. =   9
 NUMBER OF d-PARAMETER ESTIMATES SET TO MIN. OR MAX =   3

 MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

            Last Value of Negative Log Likelihood:  0.21936595D+03
            New Value of Negative Log Likelihood:   0.21769968D+03
                                     Difference:  0.16662630D+01

                 Phase Converged by Criterion of: +/-    5.5

 Step Not Converged: Convergence for  1 Successive Phase(s)
```

****

Start of Phase #   2

Theta Estimation: Convergence reached for   47 Cases in 16 Iteration(s)

NUMBER OF PROFICIENCY ESTIMATES SET TO MIN. OR MAX. =   3

MAXIMUM # ITERATIONS REACHED BEFORE TOTAL CONVERGENCE

```
Last Value of Negative Log Likelihood:  0.21769968D+03
New Value of Negative Log Likelihood:   0.21216313D+03
                          Difference:  0.55365539D+01

     -Ln(Likelihood) after Rescaling:        0.21504503D+03

     Phase Converged by Criterion of: +/-    5.5
```

Step Converged: Two Successive Phases Converged

FINAL ITEM PARAMETER AND STANDARD ERROR ESTIMATES

			Dimension 1		Dimension 2	
Item	d	S.E.	a1	S.E.	a2	S.E.
1	1.849	0.516	4.500*	0.677	4.500*	0.655
2	2.122	0.450	0.909	0.428	0.143	0.326
3	-3.063	0.577	0.064	0.540	1.251	0.370
4	0.811	0.378	1.601	0.445	1.924	0.474
5	1.986	0.462	0.010*	0.484	3.986	0.872
6	1.360	0.382	1.107	0.407	0.861	0.385
7	-1.378	0.463	0.010*	0.525	4.500*	1.562
8	-4.500*	0.583	3.400c	0.522	4.500*	0.633
9	1.683	0.487	0.983	0.581	4.500*	0.973
10	0.229	0.428	3.461	0.845	0.384	0.380
11	-0.655	0.344	1.764	0.428	0.718	0.316
12	1.088	0.378	0.010*	0.404	2.470	0.691
13	-4.500*	0.628	2.429	0.544	3.801	0.584
14	-4.500*	0.573	3.319	0.493	0.617	0.533
15	2.843c	0.578	4.500*	0.772	1.329c	0.503

m Indicates value set to maximum or minimum (before rescaling)
c Indicates estimate did not converge
* Indicates no convergence AND set to maximum or minimum

MULTIDIMENSIONAL ITEM PARAMETER ESTIMATES

Item	Gamma (MDISC)	Beta (MDIF)	Alphas (Angles) Dim. 1	Dim. 2
1	6.364	-0.291	45.000	45.000
2	0.920	-2.306	8.908	81.092
3	1.253	2.445	87.064	2.936
4	2.504	-0.324	50.236	39.764
5	3.986	-0.498	89.852	0.148
6	1.403	-0.970	37.857	52.143
7	4.500	0.306	89.869	0.131
8	5.640	0.798	52.928	37.072
9	4.606	-0.365	77.678	12.322
10	3.482	-0.066	6.333	83.667
11	1.905	0.344	22.149	67.851
12	2.470	-0.440	89.761	0.239
13	4.511	0.998	57.419	32.581
14	3.376	1.333	10.532	79.468
15	4.692	-0.606	16.448	73.552

FINAL THETA AND STANDARD ERROR ESTIMATES

	Dimension 1		Dimension 2	
Case	Th 1	S.E.	Th 2	S.E.
1	0.967,	0.404	0.294	0.263
2	-0.632	0.289	0.487	0.291
3	-0.312	0.293	0.128	0.259
4	-0.070	0.296	-0.160	0.244
5	-1.829	0.431	2.994	0.485
6	0.622	0.390	-0.649	0.264
7	-2.043	0.444	2.049	0.402
8	-0.316	0.303	0.198	0.267
9	1.001	0.399	0.289	0.261
10	-0.436	0.284	-0.234	0.244
11	0.011	0.289	-0.409	0.234
12	-0.536	0.284	-0.129	0.246
13	-0.602	0.354	1.030	0.456
14	-0.750	0.449	-0.753	0.375
15	-0.726	0.333	1.856	0.332
16	-1.405	0.464	0.532	0.319
17	0.925	0.486	0.011	0.298
18	0.107	0.311	-0.763	0.281
19	1.159	0.513	-0.649	0.286
20	0.423	0.488	0.069	0.313
21	1.345	0.371	0.195	0.252
22	-0.253	0.779	-4.275*	3.093
23	-0.680	0.337	0.916	0.440
24	0.458	0.418	0.570	0.303
25	1.707	0.392	-0.221	0.259
26	0.630	0.427	-1.523	0.521
27	-0.439	0.272	0.058	0.244
28	1.130	0.496	-0.266	0.294
29	1.573	0.378	-0.061	0.258
30	-0.349	0.286	0.118	0.254
31	-0.474	0.281	0.234	0.257
32	0.113	0.395	0.088	0.299
33	-0.351	0.336	1.538	0.328
34	-0.011	0.622	4.444*	2.228
35	-1.559	0.472	4.444*	1.352

36	0.172	0.299	-0.498	0.237
37	0.175	0.389	-0.040	0.288
38	-2.411	1.226	-0.150	0.320
39	1.130	0.496	-0.266	0.294
40	-0.344	0.276	0.017	0.245
41	-2.012	1.256	-0.469	0.356
42	-0.812	0.319	1.518	0.347
43	0.227	0.333	-2.827	1.148
44	1.527	0.351	-1.655	0.404
45	1.125	0.408	-1.137	0.365
46	1.361	0.355	-1.901	0.401
47	-0.343	0.324	-0.742	0.333
48	0.840	0.535	-0.210	0.304
49	1.111	0.384	0.279	0.256
50	-0.146	0.343	0.243	0.291

---

m Indicates value set to maximum or minimum (before rescaling)
c Indicates estimate did not converge
* Indicates no convergence AND set to maximum or minimum
P Indicates PERFECT No. right Score for this Case
Z Indicates ZERO No. Right Score for this Case

Correlations Among Theta Estimates (or Thetas when Fixed)

	Theta(01)	Theta(02)
Theta(01)	1.000	
Theta(02)	-0.395	1.000

Variances of Residuals for Each Item & Covariances of Residuals with Theta Estimates (or thetas) & the Other Items

---

Item Number 1 : Residual Variance = 0.069

Covariances with Thetas: 0.011 0.003

Residual Covariances (Item # : Cov.)

2:	0.019	3:	0.017	8:	0.000	13:	-0.002	14:	-0.002
7:	-0.009	4:	-0.009	5:	-0.010	12:	-0.010	10:	-0.013
9:	-0.027	6:	-0.029	11:	-0.031	15:	-0.033		

Item Number 2 : Residual Variance = 0.105

Covariances with Thetas: -0.023 0.011

Residual Covariances (Item # : Cov.)

1:	0.019	5:	0.014	3:	0.007	8:	0.005	12:	0.004
7:	0.003	10:	0.001	14:	0.000	13:	-0.002	11:	-0.009
15:	-0.017	9:	-0.019	4:	-0.031	6:	-0.037		

Item Number 3 : Residual Variance = 0.062

Covariances with Thetas: 0.019 -0.035

Residual Covariances (Item # : Cov.)

10:	0.018	1:	0.017	2:	0.007	5:	0.007	14:	0.002
8:	0.000	4:	-0.003	11:	-0.003	13:	-0.004	6:	-0.008
7:	-0.009	12:	-0.010	9:	-0.011	15:	-0.023		

Item Number 4 : Residual Variance = 0.154

Covariances with Thetas: 0.023 -0.033

Residual Covariances (Item # : Cov.)

11:	0.024	6:	0.006	13:	0.005	5:	-0.001	3:	-0.003
14:	-0.003	7:	-0.007	15:	-0.008	1:	-0.009	8:	-0.013
12:	-0.013	9:	-0.027	2:	-0.031	10:	-0.033		

Item Number 5 : Residual Variance = 0.108

Covariances with Thetas: 0.001 -0.017

Residual Covariances (Item # : Cov.)

6:	0.050	2:	0.014	15:	0.013	3:	0.007	13:	0.003
10:	0.002	4:	-0.001	14:	-0.002	1:	-0.010	8:	-0.011
9:	-0.019	11:	-0.022	7:	-0.042	12:	-0.049		

Item Number 6 : Residual Variance = 0.137

Covariances with Thetas: 0.026 -0.047

Residual Covariances (Item # : Cov.)

5:	0.050	15:	0.013	9:	0.012	10:	0.011	13:	0.009
4:	0.006	14:	0.001	12:	-0.004	3:	-0.008	8:	-0.019
11:	-0.023	1:	-0.029	7:	-0.032	2:	-0.037		

Item Number 7 : Residual Variance = 0.060

Covariances with Thetas: -0.026 0.021

Residual Covariances (Item # : Cov.)

11:	0.035	10:	0.010	13:	0.010	14:	0.004	2:	0.003
12:	-0.001	15:	-0.002	4:	-0.007	8:	-0.009	1:	-0.009
3:	-0.009	9:	-0.009	6:	-0.032	5:	-0.042		

Item Number 8 : Residual Variance = 0.039

Covariances with Thetas: -0.020 0.031

Residual Covariances (Item # : Cov.)

9:	0.009	2:	0.005	1:	0.000	3:	0.000	10:	-0.001
15:	-0.002	12:	-0.006	7:	-0.009	14:	-0.010	11:	-0.011
5:	-0.011	4:	-0.013	6:	-0.019	13:	-0.021		

Item Number 9 : Residual Variance = 0.073

Covariances with Thetas: 0.003 0.004

Residual Covariances (Item # : Cov.)

10:	0.021	6:	0.012	8:	0.009	15:	0.008	14:	0.003
11:	0.000	12:	-0.009	7:	-0.009	3:	-0.011	13:	-0.017
5:	-0.019	2:	-0.019	4:	-0.027	1:	-0.027		

Item Number 10 : Residual Variance = 0.095

Covariances with Thetas: 0.016 0.000

Residual Covariances (Item # : Cov.)

9:	0.021	3:	0.018	6:	0.011	7:	0.010	5:	0.002
2:	0.001	14:	0.001	8:	-0.001	12:	-0.003	13:	-0.004
11:	-0.009	1:	-0.013	4:	-0.033	15:	-0.048		

Item Number 11 : Residual Variance = 0.171

Covariances with Thetas: 0.013 -0.003

Residual Covariances (Item # : Cov.)

7:	0.035	4:	0.024	12:	0.009	9:	0.000	3:	-0.003
14:	-0.005	10:	-0.009	2:	-0.009	13:	-0.010	8:	-0.011
15:	-0.016	5:	-0.022	6:	-0.023	1:	-0.031		

Item Number 12 : Residual Variance = 0.131

Covariances with Thetas: -0.032 0.010

Residual Covariances (Item # : Cov.)

14:	0.018	11:	0.009	15:	0.008	2:	0.004	13:	0.002
7:	-0.001	10:	-0.003	6:	-0.004	8:	-0.006	9:	-0.009
3:	-0.010	1:	-0.010	4:	-0.013	5:	-0.049		

Item Number 13 : Residual Variance = 0.038

Covariances with Thetas: -0.016 -0.068

Residual Covariances (Item # : Cov.)

7:	0.010	6:	0.009	15:	0.008	4:	0.005	5:	0.003
14:	0.003	12:	0.002	1:	-0.002	2:	-0.002	10:	-0.004
3:	-0.004	11:	-0.010	9:	-0.017	8:	-0.021		

Item Number 14 : Residual Variance = 0.025

Covariances with Thetas: -0.106 0.007

Residual Covariances (Item # : Cov.)

12:	0.018	7:	0.004	9:	0.003	13:	0.003	3:	0.002
6:	0.001	10:	0.001	2:	0.000	15:	-0.001	5:	-0.002
1:	-0.002	4:	-0.003	11:	-0.005	8:	-0.010		

Item Number 15 : Residual Variance = 0.075

Covariances with Thetas: 0.007 0.007

Residual Covariances (Item # : Cov.)

5:	0.013	6:	0.013	13:	0.008	9:	0.008	12:	0.008
14:	-0.001	8:	-0.002	7:	-0.002	4:	-0.008	11:	-0.016
2:	-0.017	3:	-0.023	1:	-0.033	10:	-0.048		

Distribution of Residual Covariances

Range	Frequency
< .011	64
.011 - .012	5
.013 - .014	6
.015 - .016	1
.017 - .018	5
.019 - .020	4
.021 - .030	9
.031 - .040	7
.041 - .050	4
.051 - .060	0
.061 - .070	0
.070 <	0

Note: Ranges in Second Half of Table Larger than in First Half

History of -Ln(Likelihood) Function

Step	Phase	-Ln(Like)	Change
0	0	0.326581D+03	
1	1	0.287870D+03	0.387103D+02
1	2	0.288743D+03	-0.872252D+00
1	3	0.287644D+03	0.109922D+01
2	1	0.265513D+03	0.221308D+02
2	2	0.245909D+03	0.196041D+02
2	3	0.232578D+03	0.133308D+02
2	4	0.223861D+03	0.871649D+01
2	5	0.220146D+03	0.371579D+01
2	6	0.217627D+03	0.251855D+01
3	1	0.220469D+03	-0.284194D+01
3	2	0.219366D+03	0.110303D+01
4	1	0.217700D+03	0.166626D+01
4	2	0.215045D+03	0.265465D+01

Note: If Two Successive Phases have Changes that are Within +/- the Phase Criterion (5.50) of zero, the Phase is Defined to be Converged

Execution Halted Because Of:

Maximum Number of Steps Reached

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