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MINUIT

Function Minimization and Error Analysis

Reference Manual

Version 94.1

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MINUIT – Function Minimization and Error Analysis

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Foreword

What Minuit is intended to do.

Minuit is conceived as a tool to find the minimum value of a multi-parameter function and analyze the shape of the function around the minimum. The principal application is foreseen for statistical analysis, working on chisquare or log-likelihood functions, to compute the best-fit parameter values and uncertainties, including correlations between the parameters. It is especially suited to handle difficult problems, including those which may require guidance in order to find the correct solution.

What Minuit is not intended to do.

Although Minuit will of course solve easy problems faster than complicated ones, it is not intended for the repeated solution of identically parametrized problems (such as track fitting in a detector) where a specialized program will in general be much more efficient.

Further remarks.

In this manual examples are in monotype face and strings to be input by the user are underlined. In the index the page where a routine is defined is in **bold**, page numbers where a routine is referenced are in normal type. In the description of the routines a * following the name of a parameter indicates that this is an **output** parameter. If another * precedes a parameter in the calling sequence, the parameter in question is both an **input** and **output** parameter.

This document has been produced using L^AT_EX [1] with the cernman style option, developed at CERN. A compressed PostScript file `minuit.ps.gz`, containing a complete printable version of this manual, can be obtained from any CERN machine by anonymous ftp as follows (commands to be typed by the user are underlined):

```
ftp asis01.cern.ch
Trying 128.141.201.136...
Connected to asis01.cern.ch.
220 asis01 FTP server (Version 6.10 ...) ready.
Name (asis01:username): anonymous
Password: your_mailaddress
230 Guest login ok, access restrictions apply.
ftp> cd cernlib/doc/ps.dir
ftp> get minuit.ps
ftp> quit
```

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Chapter 1: Minit Basic Concepts

1.1 The Organization of Minit.

The Minit package acts on a multiparameter Fortran function to which we give the generic name FCN, although the actual name may be chosen by the user. This function must be defined and supplied by the user (or by an intermediate program such as HBOOK[2] or PAW[3], in case Minit is being used under the control of such an intermediate program). The value of FCN will in general depend on one or more variable parameters whose meaning is defined by the user (or by the intermediate program), but whose trial values are determined by Minit according to what the user requests should be done to FCN (usually minimize it).

To take a simple example, suppose the problem is to fit a polynomial through a set of data points. Then the user would write an FCN which calculates the chisquare between a polynomial and the data; the variable parameters of FCN would be the coefficients of the polynomials. Using Minit commands, the user would request Minit to minimize FCN with respect to the parameters, that is, find those values of the coefficients which give the lowest value of chisquare.

The user must therefore supply, in addition to the function to be analyzed, a set of commands to instruct Minit what analysis is wanted. The commands may be given in several different forms:

- As a data file, corresponding to the traditional “data cards”, for batch processing;
- Typed in at execution time at a terminal, for interactive running;
- Coded in Fortran in the calling program, which allows looping, conditional execution, and all the other possibilities of Fortran, but not interactivity, since it must be compiled before execution. This is sometimes known as running Minit in “slave mode”. HBOOK and PAW use Minit in this way.

It is also possible to mix any of the above forms, for example starting off a fit with a standard command file, then turning it over to the interactive user for the final command steps.

1.2 Internal and External Parameters.

Each of the parameters to FCN is defined by the user as belonging to one of the following types:

- | | |
|------------------------------|---|
| Freely variable: | allowed to take on any value. |
| Variable with limits: | allowed to vary only between two limits specified by the user. |
| Fixed: | originally defined as variable, but now taking on only the value the parameter had at the moment it was fixed, or a value later assigned by the user. |
| Constant: | taking on only one value as specified by the user. |
| Undefined: | never defined by user. |

The user, in FCN, must of course be able to “see” all types of defined parameters, and he therefore has access to what we call the *external parameter list*, that is, the parameters as he defined them. On the other hand, the internal Minit minimizing routines only want to “see” variable parameters without limits, and so they have access only to the *internal parameter list* which is created from the external list by the following transformation:

- 1 Squeeze out all parameters that are not variable.
- 2 Transform all variable parameters with limits, so that the transformed parameter can vary without limits. (See the next section for details concerning this transformation.) Because this transformation is non-linear, it is recommended to avoid putting limits on parameters where they are not needed.

As an example, suppose that the user has defined the following parameters:

- Parameter 1, constant.
- Parameter 3, freely variable.
- Parameter 10, variable with limits.
- Parameter 11, constant.
- Parameter 22, freely variable.
- All others undefined.

Then the internal parameter list would be as follows:

- Internal parameter 1 = external parameter 3.
- Internal parameter 2 = external parameter 10, transformed appropriately.
- Internal parameter 3 = external parameter 22.

In the above example, Minuit considers that the number of external parameters is 22 (the highest external parameter number defined), and the number of internal parameters is 3. The latter number is passed as NPAR to FCN. This is the number which determines, for example, the size of the error matrix of the parameters, since only variable parameters have errors.

An important feature of Minuit is that parameters are allowed to change types during a Minuit run. Several Minuit commands are available to make variable parameters fixed and vice-versa; to impose, change, or remove limits from variable parameters; and even to define completely new parameters at any time during a run. In addition, some Minuit routines (notably the MINOS error analysis) cause one or more variable parameters to be temporarily fixed during the calculation. Therefore, the correspondence between external and internal parameter lists is in general a dynamic one, and the value of NPAR is not necessarily constant.

1.2.1 The transformation for parameters with limits.

For variable parameters with limits, Minuit uses the following transformation:

$$P_{\text{int}} = \arcsin \left(2 \frac{P_{\text{ext}} - a}{b - a} - 1 \right) \qquad P_{\text{ext}} = a + \frac{b - a}{2} (\sin P_{\text{int}} + 1)$$

so that the internal value P_{int} can take on any value, while the external value P_{ext} can take on values only between the lower limit a and the upper limit b . Since the transformation is necessarily non-linear, it would transform a nice linear problem into a nasty non-linear one, which is the reason why limits should be avoided if not necessary. In addition, the transformation does require some computer time, so it slows down the computation a little bit, and more importantly, it introduces additional numerical inaccuracy into the problem in addition to what is introduced in the numerical calculation of the FCN value. The effects of non-linearity and numerical roundoff both become more important as the external value gets

closer to one of the limits (expressed as the distance to nearest limit divided by distance between limits). The user must therefore be aware of the fact that, for example, if he puts limits of $(0, 10^{10})$ on a parameter, then the values 0.0 and 1.0 will be indistinguishable to the accuracy of most machines.

The transformation also affects the parameter error matrix, of course, so Minuit does a transformation of the error matrix (and the “parabolic” parameter errors) when there are parameter limits. Users should however realize that the transformation is only a linear approximation, and that it cannot give a meaningful result if one or more parameters is very close to a limit, where $\partial P_{\text{ext}}/\partial P_{\text{int}} \approx 0$. Therefore, it is recommended that:

- Limits on variable parameters should be used only when needed in order to prevent the parameter from taking on unphysical values.
- When a satisfactory minimum has been found using limits, the limits should then be removed if possible, in order to perform or re-perform the error analysis without limits.

Further discussion of the effects of parameter limits may be found in the last chapter.

1.3 Minuit Strategy.

At many places in the analysis of the user function, Minuit must decide whether to be “safe” and waste a few function calls in order to know where it is, or to be “fast” and attempt to get the requested results with the fewest possible calls at a certain risk of not obtaining the precision desired by the user. In order to allow the user to influence these decisions, there is an internal Minuit parameter ISTRAT which can be set by the user through the command SET STRategy. In the current release, this parameter can take on three integer values (0, 1, 2), and the default value is 1. Value 0 indicates to Minuit that it should economize function calls; it is intended for cases where there are many variable parameters and/or the function takes a long time to calculate and/or the user is not interested in very precise values for parameter errors. On the other hand, the value 2 indicates that Minuit is allowed to waste function calls in order to be sure that all values are precise; it is intended for cases where the function is evaluated in a very short time and/or where the parameter errors must be calculated reliably

1.4 Parameter Errors.

Minuit is usually used to find the “best” values of a set of parameters, where “best” is defined as those values which minimize a given function, FCN. The width of the function minimum, or more generally, the shape of the function in some neighbourhood of the minimum, gives information about the *uncertainty* in the best parameter values, often called by physicists the *parameter errors*. An important feature of Minuit is that it offers several tools to analyze the parameter errors.

1.4.1 FCN Normalization and the ERRor definition.

Whatever method is used to calculate the parameter errors, they will depend on the overall (multiplicative) normalization of FCN, in the sense that if the value of FCN is everywhere multiplied by a constant β , then the errors will be decreased by a factor $\sqrt{\beta}$. Additive constants do not change the parameter errors, but may imply a different goodness-of-fit confidence level.

Assuming that the user knows what the normalization of his FCN means, and also that he is interested in parameter errors, the SET ERRordef command allows him to define what he means by one “error”, in terms of the change in FCN value which should be caused by changing one parameter by one “error”.

If the FCN is the usual chisquare function (defined below), then `ERRORDEF` should be set to 1.0 (the default value anyway) if the user wants the usual one-standard-deviation errors. If FCN is a negative-log-likelihood function, then the one-standard-deviation value for `ERRORDEF` is 0.5. If FCN is a chisquare, but the user wants two-standard-deviation errors, then `ERRORDEF` should be = 4.0, etc.

Note that in the usual case where Minuit is being used to perform a fit to some experimental data, the parameter errors will be proportional to the uncertainty in the data, and therefore meaningful parameter errors cannot be obtained unless the measurement errors of the data are known. In the common case of a least-squares fit, FCN is usually defined as a chisquare:

$$\chi^2(\alpha) = \sum_{i=1}^n \frac{f(x_i, \alpha) - e_i)^2}{\sigma_i^2} \quad (1.1)$$

where α is the vector of free parameters being fitted, and the σ_i are the uncertainties in the individual measurements e_i . If these uncertainties are not known, and are simply left out of the calculation, then the fit may still have meaning, but not the quantitative values of the resulting parameter errors. (Only the relative errors of different parameters with respect to each other may be meaningful.)

If the σ_i are all overestimated by a factor β , then the resulting parameter errors from the fit will be overestimated by the same factor β .

1.4.2 The Error Matrix.

The Minuit processors `MIGRAD` and `HESSE` normally produce an error matrix. This matrix is the inverse of the matrix of second derivatives of FCN, transformed if necessary into external coordinate space¹, and multiplied by the square root of `ERRORDEF`. Therefore, errors based on the Minuit error matrix take account of all the parameter correlations, but not the non-linearities. That is, from the error matrix alone, two-standard-deviation errors are always exactly twice as big as one-standard-deviation errors.

When the error matrix has been calculated (for example by the successful execution of a command `MIGrad` or `HESse`) then the parameter errors printed by Minuit are the square roots of the diagonal elements of this matrix. The commands `SHOW COVariance` and `SHOW CORrelations` allow the user to see the off-diagonal elements as well. The command `SHOW EIGenvalues` causes Minuit to calculate and print out the eigenvalues of the error matrix, which should all be positive if the matrix is positive-definite (see below on `Migrad` and positive-definiteness).

The effect of correlations on the individual parameter errors can be seen as follows. When parameter `N` is `FIXed`, Minuit inverts the error matrix, removes the row and column corresponding to parameter `N`, and re-inverts the result. The effect on the errors of the other parameters will in general be to make them smaller, since the component due to the uncertainty in parameter `N` has now been removed. (In the limit that a given parameter is uncorrelated with parameter `N`, its error will not change when parameter `N` is fixed.) However the procedure is not reversible, since Minuit forgets the original error matrix, so if parameter `N` is then `RELeased`, the error matrix is considered as unknown and has to be recalculated with appropriate commands.

¹The *internal error matrix* maintained by Minuit is transformed for the user into *external coordinates*, but the numbering of rows and columns is of course still according to internal parameter numbering, since one does not want rows and columns corresponding to parameters which are not variable. The transformation therefore affects only parameters with limits; if there are no limits, internal and external error matrices are the same.

1.4.3 MINOS Errors.

The Minuit processor MINOS was probably the first, and may still be the only, generally available program to calculate parameter errors taking into account both parameter correlations and non-linearities. The MINOS error intervals are in general asymmetric, and may be expensive to calculate, especially if there are a lot of free parameters and the problem is very non-linear.

MINOS can only operate after a good minimum has already been found, and the error matrix has been calculated, so the MINOS command will normally follow a MIGRAD command. The MINOS error for a given parameter is defined as the change in the value of that parameter which causes F' to increase by the amount UP, where F' is the minimum of FCN with respect to all *other* free parameters, and UP is the ERRORDEF value specified by the user (default = 1.).

The algorithm for finding the positive and negative MINOS errors for parameter N consists of varying parameter N, each time minimizing FCN with respect to all the other NPAR-1 variable parameters, to find numerically the two values of parameter N for which the minimum of FCN takes on the values FMIN+UP, where FMIN is the minimum of FCN with respect to all NPAR parameters. In order to make the procedure as fast as possible, MINOS uses the error matrix to predict the values of all parameters at the various sub-minima which it will have to find in the course of the calculation, and in the limit that the problem is nearly linear, the predictions of MINOS will be nearly exact, requiring very few iterations. On the other hand, when the problem is very non-linear (i.e., FCN is far from a quadratic function of its parameters), that is precisely the situation when MINOS is needed in order to indicate the correct parameter errors.

1.4.4 Contour Plotting

Minuit currently offers two very different procedures for finding FCN contours. They will be identified by the corresponding command names: CONtour and MNContour.

CONtour

This procedure is designed for a lineprinter or alphanumeric terminal as output device, and gives a static picture of FCN as function of the two parameters specified by the user, that is, all the other variable parameters (if any) are considered as temporarily fixed at their current values. First a range is chosen, by default two current standard deviations on either side of the current best value of each of the two parameters, and a grid size n is chosen, by default 25 by 25 positions for the full range of each parameter. Contour zero is defined as the current best function value F_{\min} (presumably the minimum), and then the i^{th} contour is defined as where FCN has the value $F_{\min} + i^2 * UP$. The procedure then simply evaluates FCN at the four corners of each of the n^2 grid positions (which makes $(n + 1)^2$ evaluations) to determine whether the i^{th} contour passes through it. The method, although not very efficient or precise, is very robust, and capable of revealing unexpected multiple valleys.

MNContour

The contour calculated by MNContour is dynamic, in the sense that it represents the minimum of FCN with respect to all the other NPAR-2 parameters (if any). In statistical terms, this means that MNContour takes account of the correlations between the two parameters being plotted, and all the other variable parameters, using a procedure analogous to that of MINOS. (If this feature is not wanted, then the other parameters must be FIXED before calling MNContour.) MNContour provides the actual coordinates of the points around the contour, suitable for plotting with a graphics routine or by hand. The points are given

in counter-clockwise order around the contour. Only one contour is calculated per command (or Fortran call), and the level is $F_{\min} + UP$, where UP is the `ERRordef` specified by the user, or 1.0 by default. The number of points to be calculated is chosen by the user (Default is 20 for the data-driven mode.). As a by-product, `MNContour` provides the `MINOS` errors of the two parameters in question, since these are just the extreme points of the contour (Use `SHOW MINOS` to see them). In command-driven mode, a rough (alphanumeric, not graphic) plot of the points is given (if `PRIntlevel` ≥ 0) and the numerical values of the coordinates are printed (if `PRIntlevel` ≥ 1). In Fortran-callable mode, the user gets Fortran access to the vector of point coordinates through `SUBROUTINE MNCONT`.

Chapter 2: Minuit Installation.

2.1 Minuit Releases.

Minuit has been extensively revised in 1989, but the usage is largely compatible with that of older versions which have been in use since before 1970. Users familiar with older releases, who have not yet used releases from 1989 or later, must however read this manual, in order to adapt to the few changes as well as to discover the new features and easier ways of using old features, such as free-field input.

2.2 Minuit Versions.

The program is entirely in standard portable Fortran 77, and requires no external subroutines except those defined as part of the Fortran 77 standard and one logical function INTRAC¹. The only difference between versions for different computers, apart from INTRAC, is the floating point precision (see heading below).

As with previous releases, Minuit does not use a memory manager. This makes it easy to install and independent of other programs, but has the disadvantage that both the memory occupation and the maximum problem size (number of parameters) are fixed at compilation time. The old solution to this problem, which consisted of providing “long” and “short” versions, has proved to be somewhat clumsy and anyway insufficient for really exceptional users, so it has been abandoned in favour of a single “standard” version.

The currently “standard” version of Minuit will handle functions of up to 100 parameters, of which not more than 50 can be variable at one time. Because of the use of the PARAMETER statement in the Fortran source, redimensioning for larger (or smaller) versions is very easy (although it will help to have a source code manager or a good editor to propagate the modified PARAMETER statement through all the subroutines, and of course it implies recompilation). The definition of what is “standard” may well change in the light of experience (it was 35 instead of 50 variable parameters for release 89.05), and it is likely that different installations will wish to define it differently according to their own applications. In any case, the dimensions used at compilation time are printed in the program header at execution time, and the program is of course protected against the user trying to define too many parameters. The user who finds that the version available to him is too small (or too big) must try to convince his computer manager to change the installation default or to provide an additional special version, or else he must obtain the source and recompile his own version.

2.3 Interference with Other Packages

The new Minuit has been designed to interfere as little as possible with other programs or packages which may be loaded at the same time. Thus it uses no memory manager or other external subroutines (except LOGICAL FUNCTION INTRAC), all its own subroutine names start with the letters MN (except Minuit and the user written routines), all COMMON block names start with the characters MN7, and the user should not need to use explicitly any Minuit COMMON blocks.

In addition, more than one different functions can be minimized in the same execution module, provided the functions have different names, and provided one minimization and error analysis is completely finished before the next one begins.

¹INTRAC is available from the CERN Program Library for all common computers, and in the worst case can be replaced by a LOGICAL FUNCTION returning a value of .TRUE. or .FALSE. depending on whether or not Minuit is being used interactively.

2.4 Floating-point Precision

It is recommended for most applications to use 64-bit floating point precision, or the nearest equivalent on any particular machine. This means that the standard Minuit installed on Vax, IBM and Unix workstations will normally be the `DOUBLE PRECISION` version, while on CDC and Cray it will be `SINGLE PRECISION`.

The arguments of the user's FCN must of course correspond in type to the declarations compiled into the Minuit version being used. The same is true of course for all floating-point arguments to any Minuit routines called directly by the user in Fortran-callable mode. Furthermore, Minuit detects at execution time the precision with which it was compiled, and expects that the calculations inside FCN will be performed approximately to the same accuracy. (This accuracy is called EPSMAC and is printed in the header produced by Minuit when it begins execution.) If the user fools Minuit by using a double precision version but making internal FCN or FUTIL computations in single precision, Minuit will interpret roundoff noise as significant and will usually either fail to find a minimum, or give incorrect values for the parameter errors. It is therefore recommended, when using double precision (`REAL*8`) Minuit, to make sure all computations in FCN and FUTIL (if used), as well as all subroutines called by FCN and FUTIL, are `REAL*8`, by including the appropriate `IMPLICIT` declarations in FCN and all user subroutines called by FCN. If for some reason the computations cannot be done to a precision comparable with that expected by Minuit, the user **must** inform Minuit of this situation with the `SET EPS` command.

Although 64-bit precision is recommended in general, the new Minuit is so careful to use all available precision that in many cases, 32 bits will in fact be enough. It is therefore possible now to envisage in some situations (for example on microcomputers or when memory is severely limited, or if 64-bit arithmetic is very slow) the use of Minuit with 32- or 36-bit precision. With reduced precision, the user may find that certain features sensitive to first and second differences (`HESse`, `MINOs`, `MNContour`) do not work properly, in which case the calculations must be performed in higher precision.

Chapter 3: How to Use Minuit

3.1 The Function FCN.

The user must always supply a Fortran subroutine which calculates the function value to be minimized or analyzed.

```
CALL FCN (NPAR, GRAD, FVAL, XVAL, IFLAG, FUTIL)
```

Input parameters

NPAR number of currently variable parameters.
XVAL vector of (constant and variable) parameters.
IFLAG Indicates what is to be calculated (see example below).
FUTIL Name of utility routine (if needed, it must be declared EXTERNAL and provided by the user).

Output parameters

FVAL The calculated function value.
GRAD The (optional) vector of first derivatives).

Note that when Minuit is being used through an intermediate package such as HBOOK or PAW, then the FCN may be supplied by the this package.

Example of FCN routine

```
SUBROUTINE FCN(NPAR,GRAD,FVAL,XVAL,IFLAG,FUTIL)
IMPLICIT DOUBLE PRECISION (A-H,O-Z) ! for 32-bit machines
DIMENSION GRAD(*),XVAL(*)
EXTERNAL FUTIL ! (if needed and supplied by user)
C-
C   IF (IFLAG .EQ. 1) THEN
C       read input data,
C       calculate any necessary constants, etc.
C   ENDIF
C   IF (IFLAG .EQ. 2) THEN
C       calculate GRAD, the first derivatives of FVAL
C       (this is optional)
C   ENDIF
C       Always calculate the value of the function, FVAL,
C       which is usually a chisquare or log likelihood.
C       Optionally, calculation of FVAL may involve
C   FTHEO = FUTIL(...)
C       It is responsibility of user to pass
C       any parameter values needed by FUTIL,
C       either through arguments, or in a COMMON block
C   IF (IFLAG .EQ. 3) THEN
C       will come here only after the fit is finished.
C       Perform any final calculations, output fitted data, etc.
C   ENDIF
RETURN
END
```

The name of the subroutine may be chosen freely (in documentation we give it the generic name FCN) and must be declared EXTERNAL in the user's program which calls Minuit (in data-driven mode) or calls Minuit subroutines (in Fortran-callable mode). The meaning of the parameters XVAL is of course defined by the user, who uses the values of those parameters to calculate his function value. The starting values must be specified by the user (either by supplying parameter definitions from a file, or typing them at the terminal, in data-driven mode; or by calling subroutine MNPARM in Fortran-callable mode), and later values are determined by Minuit as it searches for the minimum or performs whatever analysis is requested by the user. FUTIL represents the name of a function or subroutine which may be defined and supplied by the user and called from FCN. If the user does not use the FUTIL feature, the last argument may be given as zero, but if used, the name of FUTIL must be declared EXTERNAL and a subprogram of that name must be supplied at loading time.

It is possible, by giving them different names, to analyze several different FCNs in one job. However, one analysis must be completed before the next is started. In order to avoid interference between the analyses of two different FCNs, the user should call Minuit (in data-driven mode) or MNINIT (in Fortran-callable mode) each time a new FCN is to be studied.

3.2 Running Minuit in Data-driven Mode.

Minuit can be run in two different modes: **Data-driven mode** means that the user drives Minuit with data, either typed interactively from a terminal or from a data file in batch; and **Fortran-callable mode** means that Minuit is driven directly from Fortran subroutine calls, without data. To some extent, the two modes may also be mixed. This section describes the first mode, and is valid for both interactive and batch running. The differences between interactive and batch are described in a separate subsection below.

In **data-driven mode**, the user must supply, in addition to the subroutine FCN, a **main program** which includes the following statements (the statements in upper case are required, those given in lower case are optional):

Example of main program when using Minuit in data driven mode

```
EXTERNAL FCN
external futil
call mintio(ird,iwr,isav)
CALL MINUIT(FCN,futil)
```

The name of FCN may be chosen freely, and is communicated to Minuit as its first argument. FUTIL is the generic name of a function or subroutine which the user may optionally call from FCN, and if he does call such a routine, he must declare it external and communicate its name to Minuit as well. If FUTIL is not used, then the second argument may be put equal to 0, and need not be declared EXTERNAL; if FUTIL is declared EXTERNAL, it must be supplied in the loading process.


```
CALL MINTIO (IREAD,IWRITE,ISAVE)
```

Action: The purpose of MINTIO is to communicate to Minuit the I/O units.

Input parameters

IREAD Fortran unit number for reading (default 5).

IWRITE Fortran unit number for writing (default 6).

Isave Fortran unit number for saving (default 7).

If the default values are acceptable, then it is not necessary to call MINTIO. It is the user's responsibility that the I/O units are properly opened for the appropriate operations.

Note

In data-driven mode, that is with CALL MINUIT, you should **not call** MNINIT, since Minuit takes care of all initialization. To change unit numbers, call MINTIO **before calling** MINUIT.

In order that control returns to the user program after CALL MINUIT, the last command in the corresponding Data Block should be RETURN. If the last command is EXIT or STOP, then Minuit will execute a Fortran STOP, and if the last command is END, Minuit will read a new Data Block from the current input unit.

3.2.1 Data to drive Minuit

In data-driven mode, either interactively or in batch, Minuit reads the following data provided by the user:

- **Title:** (a string of 50 characters or less) which can be chosen freely by the user, to help identify the job.
- **Parameter definitions:** for each parameter one record giving:
 - 1 **The parameter number.** This is the index in the array XVAL by which the user function FCN will access the value of the parameter.
 - 2 **The parameter name.** A string of ten characters to help the user in reading the Minuit output.
 - 3 **The starting value** of the parameter.
 - 4 **The starting step size,** or expected uncertainty in this parameter, if it is to be a variable parameter. Otherwise blank or zero if the value is to be constant.

OptionalThe **lower bound** (limit) below which the parameter value must not vary.

OptionalThe **upper bound** (limit) above which the parameter value must not vary.

Normally the user should **not** specify limits on the parameters, that is both should be left blank. If one limit is specified, then BOTH must be specified. The properties of limits are explained elsewhere in this document.

The format of the parameter definitions may be either fixed-field (each item in a field of width ten columns), or in free-field format. In the free-field format, items are separated by blanks or one comma, and the parameter name must be given between single quotes. The program assumes free-field format if it finds two single quotes in the line. Parameter names will be blank-padded or truncated to be ten characters long.

- **A blank record:** indicates the end of parameter definitions.
- If the user FCN reads input data from the same input stream as the Minuit data (the default stream is UNIT 5), then the FCN data should appear here.
- **Minuit commands:** these specify actions which should be performed by Minuit. Commands must not contain leading or embedded blanks, but may be truncated to three characters, and may be given in upper or lower case. Some commands have numerical arguments, and these may be given in free-field format, separated by blank(s) or one comma¹. The list of recognized commands is given and explained below. The command HELP causes Minuit to write to the output stream a list of currently recognized commands. The command HELP SHOW lists the available SET and SHOW commands.

Any or all of the above data read by Minuit can reside on one or more different files, and Minuit can be instructed to switch to reading a different file with the SET INPUT command. Optionally, the **title** record may be preceded by a record beginning with the characters SET TITLE, and the **parameter definitions** may be preceded by a record beginning with the characters PARAMETERS. It is in fact recommended always to include these optional records when preparing a data file, since the file can then be read at any time (not just at the beginning of a Minuit run) and will always be interpreted correctly by Minuit.

Example of a typical Minuit data set

```

SET TITLE
Fit to time distribution of K decays, Expt NA94
PARAMETERS
1 'Real(X)' 0. .1
2 'Imag(X)' 0. .1
5 'Delta M' .535 .01
10 'K Short LT' .892
11 'K Long LT' 518.3

fix 5
migrad
set print 0
minos
restore
migrad
minos
fix 5
set param 5 0.535
mncontour 1 2
stop

```

3.2.2 Batch and interactive running.

In its initialization phase, Minuit attempts to determine whether or not it is running interactively, by calling the logical function INTRAC, a routine in the CERN Program Library which can be provided for all commonly used computers. For our purposes, we define “running interactively” as meaning that input is coming from a terminal under the control of an intelligent being, able to make decisions based on the

¹In older versions of Minuit, there was a special format for the MINOS command, when specifying a list of parameters; the new Minuit reads the MINOS command with the same free-field format as the other commands, so if parameter numbers are specified, they must now be separated by a blank or comma.

output he receives at the terminal. It is not always easy for INTRAC to know whether this is the case, so, depending on your operating system, Minuit can be fooled in certain cases. When this happens, the user can always override the beliefs of INTRAC with the commands `SET BATch` and `SET INTeractive`. The command `SHOw INTeractive` informs the user of the current mode.

According to whether or not it believes it is running interactively, Minuit behaves differently in the following ways:

- If interactive, the user is prompted before each data record is read.
- If interactive, Minuit recovers from many error conditions and prompts the user to enter correct data or to specify additional required input. If the same error conditions occur in batch mode, the program either exits (if no corrective action seems possible) or ignores the incorrect data (for example, a command it cannot interpret) and continues.
- The default page size for output is a typical terminal dimension (80 by 24) if interactive, and a typical printed page size (120 by 56) if batch, but these can be overridden with the commands `SET WIDth` and `SET LINes`.

When an interactive user requests Minuit to read further input from an external file (the `SET INPut` command), then further input is considered to be temporarily in batch mode, until input reverts to the primary input stream.

3.3 Running Minuit in Fortran-callable mode.

The following Minuit subroutines are provided in order to allow the user to communicate with Minuit and perform all Minuit functions (define parameters, execute commands, etc.) directly from Fortran through subroutine calls. In the following list of subroutines, output arguments are indicated by appending a star * to its name. It should also be noted that for the Double Precision version of Minuit (recommended for all 32-bit machines such as IBM, Vax, Unix workstations, etc.), all the REAL arguments given below must be declared `DOUBLE PRECISION`.

3.3.1 Initialize Minuit

```
CALL MNINIT (IRD, IWR, ISAV)
```

Input parameters:

IRD Unit number for input to Minuit.
 IWR Unit number for output from Minuit.
 ISAV Unit number for use of the SAVE command.

3.3.2 Specify a title for a problem

```
CALL MNSETI (CTITLE)
```

Input parameter:

CTITLE Character string of up to 50 characters containing an identification text for the present job or fit.

3.3.3 Define a parameter, assigning values from variables

```
CALL MNPARM (NUM, CHNAM, STVAL, STEP, BND1, BND2, IERFLG*)
```

Input parameters:

NUM Parameter number as referenced by user in FCN.

CHNAM Character string of up to 10 characters containing the name which the user assigned to the given parameter.

STVAL Starting value

STEP Starting step size or approximate parameter error.

BND1 Lower bound (limit) on parameter value, if any (see below).

BND2 Upper bound (limit) on parameter value, if any (see below).

Output parameter:

IERFLG Error return code: 0 if no error, >0 if request failed.

If BND1=BND2=0., then the parameter is considered unbounded, which is recommended unless limits are needed to make things behave well.

3.3.4 Define a parameter, assigning values from character string

Subroutine MNPARS defines a new (or redefines an old) parameter specifying values for its number, name, starting value, step size, and limits if any. All these values are given in one character string as if it was being read from the input stream. It can therefore be used in place of MNPARM if the character string format is more convenient than the calling sequence of MNPARM.

Calling sequence:

```
CALL MNPARS (CHSTR, ICONDN*)
```

Input parameter:

CHSTR String specifies the parameter definition in the usual Minuit format, as on a data record (See 3.2.1). The fields are in the same order as the arguments to MNPARM

Output parameter:

ICONDN Output condition

Possible values of output condition:

ICONDN=0 all OK

ICONDN=1 error, attempt to define parameter is ignored

ICONDN=2 end of parameter definitions (parameter number zero)

Example:

```
CALL MNPARS(' 15 ' 'Lambda Mass' ' 1.2, 0.1' , ICONDN)
```

3.3.5 Execute a Minuit command

```
CALL MNEXCM (FCN,CHCOM,ARGLIS,NARG,IERFLG*,FUTIL)
```

Input parameters:

FCN Name of the function being analyzed (to be declared EXTERNAL)
 CHCOM Character string containing the name of the Minuit command to be executed (see below).
 ARGLIS Array of dimension MAXARG, containing the numeric arguments to the command (if any),
 NARG Number of arguments specified ($NARG \leq MAXARG$),
 FUTIL Name of a function called by FCN (or =0 if not used). If used this function must be declared EXTERNAL.

Output parameter:

IERFLG Error return code: 0 if the command was executed normally, >0 otherwise.

Executing a command by calling MNEXCM has exactly the same effect as reading the same command in data-driven mode, except that a few commands would make no sense and are not available in Fortran-callable mode (e.g. SET INPUT). The other difference is that **control always returns to the calling routine from MNEXCM**, even after commands END, EXIT, and STOP.

3.3.6 Execute a Minuit command specified as a character string

Subroutine MNCOMD causes the execution of the Minuit command specified as the second argument. It therefore works like MNEXCM, except that it accepts the entire command with arguments as one character string. This is more convenient in many cases and avoids problems of word length matching (DOUBLE PRECISION constants).

```
CALL MNCOMD (FCN,CHSTR,ICONDN*,FUTIL)
```

Input parameters:

FCN Name of the function being analyzed (to be declared EXTERNAL)
 CHSTR The full Minuit command with arguments (CHARACTER)
 FUTIL Name of a function called by FCN (or =0 if not used). If used this function must be declared EXTERNAL.

Output parameter:

ICONDN Error return code: 0 if the command was executed normally, >0 otherwise.

Some abnormal conditions:

ICONDN=1 command was blank, ignored
 ICONDN=2 command line was unreadable, ignored
 ICONDN=3 command was unknown, ignored
 ICONDN=4 abnormal termination (e.g., MIGRAD not converged)

3.3.7 Get the current value of a parameter

This routine is the inverse of MNPARM and can for instance be used after a fit.

```
CALL MNPOUT (NUM, CHNAM*, VAL*, ERROR*, BND1*, BND2*, IVARBL*)
```

Input parameter:

NUM Parameter number as referenced by user in FCN and about which information is required.

Output parameters:

CHNAM Character string of up to 10 characters containing the name which the user assigned to the given parameter.

VAL Current parameter value (fitted value if fit has converged),

ERROR Current estimate of parameter uncertainty (or zero if constant)

BND1 Lower limit on parameter value, if any (otherwise zero).

BND2 Upper limit on parameter value, if any (otherwise zero).

IVARBL Internal parameter number if parameter is variable, or zero if parameter is constant, or negative if parameter is undefined.

3.3.8 Get the current status of minimization

```
CALL MNSTAT (FMIN*, FEDM*, ERRDEF*, NPARI*, NPARX*, ISTAT*)
```

Output parameters:

FMIN The best function value found so far

FEDM The estimated vertical distance remaining to minimum

ERRDEF The value of UP defining parameter uncertainties

NPARI The number of currently variable parameters

NPARX The highest (external) parameter number defined by user

ISTAT A status integer indicating how good is the covariance matrix:

0 Not calculated at all

1 Diagonal approximation only, not accurate

2 Full matrix, but forced positive-definite

3 Full accurate covariance matrix (After MIGRAD, this is the indication of normal convergence.)

3.3.9 Get the current value of the covariance matrix

```
CALL MNEMAT (EMAT*,NDIM)
```

Input parameter:

NDIM Integer variable specifying the number of rows and columns the user has reserved in EMAT to store the matrix elements. NDIM should be at least as large as the number of parameters variable at the time of the call, otherwise the user will get only part of the full matrix.

Output parameter:

EMAT Array declared as DIMENSION EMAT(NDIM,NDIM) which is to be filled with the (external) covariance matrix.

3.3.10 Access current parameter errors

```
CALL MNERRS (NUM,EPLUS*,EMINUS*,EPARAB*,GLOBCC*)
```

Input parameter:

NUM Parameter number. If NUM>0, this is taken to be an external parameter number; if NUM<0, it is the negative of an internal parameter number.

Output parameters:

EPLUS The positive MINOS error of parameter NUM.

EMINUS The negative MINOS error (a negative number).

EPARAB The “parabolic” parameter error, from the error matrix.

GLOBCC The global correlation coefficient for parameter NUM. This is a number between zero and one which gives the correlation between parameter NUM and that linear combination of all other parameters which is most strongly correlated with NUM.

Note that this call does not cause the errors to be calculated, it merely returns the current existing values. If any of the requested values has not been calculated, or has been destroyed (for example, by a redefinition of parameter values) MNERRS returns a value of zero for that argument. Thus the call to MNERRS will normally follow the execution of commands MIGRAD, HESSE, MNContour, and/or MINOS.

3.3.11 Find a function contour with the MNContour method

```
CALL MNCNT (FCN,NUM1,NUM2,NPT,XPT*,YPT*,NFOUND*,FUTIL)
```

Input parameters:

FCN Name of the function being treated (to be declared EXTERNAL)

NUM1/2 Parameter numbers with respect to which the contour is to be determined (external).

NPT The number of points required on the contour (>4).

FUTIL Name of a function called by FCN (or =0 if not used). If used this function must be declared EXTERNAL.

Output parameters:

- XPT Array of x-coordinates of contour points with values for parameter NUM1. It must be declared with a DIMENSION XPT(NPT).
- YPT Array of y-coordinates of contour points with values for parameter NUM2. It must be declared with a DIMENSION YPT(NPT).
- NFOUND The number of points actually found on the contour. If all goes well, this will be equal to NPT, but it can be negative (if the input arguments are not valid), or zero if less than four points have been found, or less than NPT if the program could not find NPT points.

Note that alternatively MNContour can be calculated by calling MNEXCM to issue the MNContour command, but then the user does not have Fortran access to the actual point coordinates XPT and YPT.

3.3.12 Switch to command-reading mode

This facility can be useful when one wants to continue interactively.

```
CALL MNINTR (FCN, FUTIL)
```

Input parameters:

- FCN Name of the function being treated (to be declared EXTERNAL)
- FUTIL Name of a function called by FCN (or =0 if not used). If used this function must be declared EXTERNAL.

The call to MNINTR will cause Minuit to read commands from the unit IRD (originally specified by the user in his call to MNINIT, IRD is usually 5 by default, which in turn is usually the terminal by default). Minuit then reads and executes commands until it encounters a command END, EXIT, RETURN, or STOP, or an end-of-file on input (or an unrecoverable error condition while reading or trying to execute a command), in which case control returns to the program which called MNINTR.

3.3.13 Set logical unit number for input

Sets logical unit number of input unit from which Minuit will read the next command.

```
CALL MNINPU (NUNIT, IERR*)
```

Input parameters:

- NUNIT The I/O unit number, which must be a valid unit, opened for reading (Minuit makes no checks at this level and will not attempt to open any files.)
- IERR returned as zero unless Minuit's internal buffer which stores unit numbers is full, which is a fatal error. If NUNIT is specified as zero, Minuit returns to reading the previous unit (which is why it has to store them).

Chapter 4: Minuit Commands

In data-driven mode, Minuit accepts commands in the following format:

```
command <arg1> [arg2] etc.
```

command One of the commands listed below,

<argi> Numerical values of **required** arguments, if any.

[argi]] Numerical values of **optional** arguments, if any.

The arguments (if any) are separated from each other and from the command by one or more blanks or a comma. Commands may be given in upper or lower case, and may be abbreviated, usually to three characters. The shortest recognized abbreviations are indicated by the capitalized part of the commands listed below. Examples of valid commands are:

```
SET INPUT 21
migrad
mig 500
SET LIMITS 14 -1.0,1.0
contours 1 2
MINOS 500 1,3,5,21,22
```

In Fortran-callable mode, all the same commands (with a few obvious exceptions as indicated) can be executed by passing the command-string and arguments to Minuit in a CALL MNEXCM statement.

List of Minuit commands

```
CAL <iflag>
```

Instructs Minuit to call subroutine FCN with the value of IFLAG=<iflag>. (The actual name of the subroutine called is that given by the user in his call to Minuit or MNEXCM; the name given in this command is not used.) If <iflag> > 5, Minuit assumes that a new problem is being redefined, and it forgets the previous best value of the function, covariance matrix, etc. This command can be used to instruct the user function to read new input data, recalculate constants, or otherwise modify the calculation of the function.

```
CLEar
```

Resets all parameter names and values to undefined. Must normally be followed by a PARAmeters command or equivalent, in order to define parameter values.

```
CONtour <par1> <par2> [devs] [ngrid]
```

Instructs Minuit to trace contour lines of the user function with respect to the two parameters whose external numbers are <par1> and <par2>. Other variable parameters of the function, if any, will have their values fixed at the current values during the contour tracing. The optional parameter [devs] (default value 2.) gives the number of standard deviations in each parameter which should lie entirely within the plotting area. Optional parameter [ngrid] (default value 25 unless page size is too small) determines the resolution of the plot, i.e. the number of rows and columns of the grid at which the function will be evaluated. [See also MNContour.]

END

Signals the end of a data block (i.e., the end of a fit), and implies that execution should continue, because another Data Block follows. A Data Block is a set of Minuit data consisting of (1) A Title, (2) One or more Parameter Definitions, (3) A blank line, and (4) A set of Minuit Commands. The END command is used when more than one Data Block is to be used with the same FCN function. CALL FCN The END command first causes Minuit to issue a CALL FCN with IFLAG=3, in order to allow FCN to perform any calculations associated with the final fitted parameter values, unless a CALL FCN 3 command has already been executed at the current FCN value. The obsolete command END RETURN is the same as the RETURN command.

EXIT

Signals the end of execution. The EXIT command first causes Minuit to issue a CALL FCN with IFLAG=3, in order to allow FCN to perform any calculations associated with the final fitted parameter values, unless a CALL FCN 3 command has already been executed at the current FCN value. Then it executes a Fortran STOP.

FIX <parno> [parno] ... [parno]

Causes parameter(s) <parno> to be removed from the list of variable parameters, and their value(s) will remain constant during subsequent minimizations, etc., until another command changes their value(s) or status.

HELP [SET] [SHOW] [command]

If there are no arguments, causes Minuit to list the available commands. If argument SET or SHOW is specified, the list of recognized SET and SHOW commands is displayed. If a command name is specified as argument, a short explanation of the command syntax is given.

HESse [maxcalls]

Instructs Minuit to calculate, by finite differences, the Hessian or error matrix. That is, it calculates the full matrix of second derivatives of the function with respect to the currently variable parameters, and inverts it, printing out the resulting error matrix. The optional argument [maxcalls] specifies the (approximate) maximum number of function calls after which the calculation will be stopped.

IMProve [maxcalls]

If a previous minimization has converged, and the current values of the parameters therefore correspond to a local minimum of the function, this command requests a search for additional distinct local minima. The optional argument [maxcalls] specifies the (approximate) maximum number of function calls after which the calculation will be stopped.

MIGrad [maxcalls] [tolerance]

Causes minimization of the function by the method of Migrad, the most efficient and complete single method, recommended for general functions (see also MINimize). The minimization produces as a by-product the error matrix of the parameters, which is usually reliable unless warning messages are produced. The optional argument [maxcalls] specifies the (approximate) maximum number of function calls after which the calculation will be stopped even if it has not yet converged. The optional argument [tolerance] specifies required tolerance on the function value at the minimum. The default tolerance is 0.1, and the minimization will stop when the estimated vertical distance to the minimum (EDM) is less than $0.001 * [tolerance] * UP$ (see SET ERR).

MINimize [maxcalls] [tolerance]

Causes minimization of the function by the method of Migrad, as does the MIGrad command, but switches to the SIMplex method if Migrad fails to converge. Arguments are as for MIGrad. Note that command requires four characters to be unambiguous with MINOs.

MINOs [maxcalls] [parno] [parno] ...

Causes a Minos error analysis to be performed on the parameters whose numbers [parno] are specified. If none are specified, Minos errors are calculated for all variable parameters. Minos errors may be expensive to calculate, but are very reliable since they take account of non-linearities in the problem as well as parameter correlations, and are in general asymmetric. The optional argument [maxcalls] specifies the (approximate) maximum number of function calls **per parameter requested**, after which the calculation will be stopped for that parameter.

MNContour <par1> <par2> [npts]

Calculates one function contour of FCN with respect to parameters par1 and par2, with FCN minimized always with respect to all other NPAR-2 variable parameters (if any). Minuit will try to find npts points on the contour (default 20). If only two parameters are variable at the time, it is not necessary to specify their numbers. To calculate more than one contour, it is necessary to SET ERR to the appropriate value and issue the MNContour command for each contour desired.

RELease <parno> [parno] ... [parno]

If <parno> is the number of a previously variable parameter which has been fixed by a command: FIX <parno>, then that parameter will return to variable status. Otherwise a warning message is printed and the command is ignored. Note that this command operates only on parameters which were at one time variable and have been FIXed. It cannot make constant parameters variable; that must be done by redefining the parameter with a PARameters command.

REStore [code]

If no [code] is specified, this command restores all previously FIXed parameters to variable status. If [code]=1, then only the last parameter FIXed is restored to variable status. If code is neither zero nor one, the command is ignored.

RETurn

Signals the end of a data block, and instructs Minuit to return to the program which called it. The RETurn command first causes Minuit to CALL FCN with IFLAG=3, in order to allow FCN to perform any calculations associated with the final fitted parameter values, unless a CALL FCN 3 command has already been executed at the current FCN value. Then it executes a Fortran RETURN.

SAVe

Causes the current parameter values to be saved on a file in such a format that they can be read in again as Minuit parameter definitions. If the covariance matrix exists, it is also output in such a format. The unit number is by default 7, or that specified by the user in his call to MINTIO or MNINIT. The user is responsible for opening the file previous to issuing the SAVE command (except where this can be done interactively).

SCAN [parno] [numpts] [from] [to]

Scans the value of the user function by varying parameter number [parno], leaving all other parameters fixed at the current value. If [parno] is not specified, all variable parameters are scanned in sequence. The number of points [numpts] in the scan is 40 by default, and cannot exceed 100. The range of the scan is by default 2 standard deviations on each side of the current best value, but can be specified as from [from] to [to]. After each scan, if a new minimum is found, the best parameter values are retained as start values for future scans or minimizations. The curve resulting from each scan is plotted on the output unit in order to show the approximate behaviour of the function. This command is not intended for minimization, but is sometimes useful for debugging the user function or finding a reasonable starting point.

SEEK [maxcalls] [devs]

Causes a Monte Carlo minimization of the function, by choosing random values of the variable parameters, chosen uniformly over a hypercube centered at the current best value. The region size is by default 3 standard deviations on each side, but can be changed by specifying the value of [devs].

SET BATCh

Informs Minuit that it is running in batch mode.

SET EPSmachine <accuracy>

Informs Minuit that the relative floating point arithmetic precision is <accuracy>. Minuit determines the nominal precision itself, but the SET EPS command can be used to override Minuit's own determination, when the user knows that the FCN function value is not calculated to the nominal machine accuracy. Typical values of <accuracy> are between 10^{-5} and 10^{-14} .

SET ERRordef <up>

Sets the value of UP (default value= 1.), defining parameter errors. Minuit defines parameter errors as the change in parameter value required to change the function value by UP. Normally, for chisquared fits UP=1, and for negative log likelihood, UP=0.5.

SET GRAdient [force]

Informs Minuit that the user function is prepared to calculate its own first derivatives and return their values in the array GRAD when IFLAG=2 (see specification of the function FCN). If [force] is not specified, Minuit will calculate the FCN derivatives by finite differences at the current point and compare with the user's calculation at that point, accepting the user's values only if they agree. If [force]=1, Minuit does not do its own derivative calculation, and uses the derivatives calculated in FCN.

SET INPut [unitno] [filename]

Causes Minuit, in data-driven mode only, to read subsequent commands (or parameter definitions or title) from a different input file. If no [unitno] is specified, reading reverts to the previous input file, assuming that there was one. If [unitno] is specified, and that unit has not been opened, then Minuit attempts to open the file [filename] if a name is specified. If running in interactive mode and [filename] is not specified and [unitno] is not opened, Minuit prompts the user to enter a file name. If the word REWIND is added to the command (note: **no blanks** between INPUT and REWIND), the file is rewound before reading. *Note that this command is implemented in standard Fortran 77 and the results may depend on the operating system; for example, if a filename is given under VM/CMS, it must be preceeded by a slash.*

SET INTeractive

Informs Minuit that it is running interactively.

SET LIMits [parno] [lolim] [uplim]

Allows the user to change the limits on one or all parameters. If no arguments are specified, all limits are removed from all parameters. If [parno] alone is specified, limits are removed from parameter [parno]. If all arguments are specified, then parameter [parno] will be bounded between [lolim] and [uplim]. Limits can be specified in either order, Minuit will take the smaller as [lolim] and the larger as [uplim]. However, if [lolim] is equal to [uplim], an error condition results.

SET LINesperpage

Sets the number of lines that Minuit thinks will fit on one page of output. The default value is 24 for interactive mode and 56 for batch.

SET NOGradient

The inverse of SET GRAdient, instructs Minuit not to use the first derivatives calculated by the user in FCN.

SET NOWarnings

Supresses Minuit warning messages. SET WARnings is the default.

SET OUTputfile <unitno>

Instructs Minuit to write further output to unit <unitno>.

SET PAGethrow <integer>

Sets the carriage control character for “new page” to <integer>. Thus the value 1 produces a new page, and 0 produces a blank line, on some output devices (see TOPofpage command).

SET PARAmeter <parno> <value>

Sets the value of parameter <parno> to <value>. The parameter in question may be variable, fixed, or constant, but must be defined.

SET PRIntout <level>

Sets the print level, determining how much output Minuit will produce. The allowed values and their meanings are displayed after a SHOW PRInt command, and are currently <level>=:

- 1 no output except from SHOW commands
- 0 minimum output (no starting values or intermediate results)
- 1 default value, normal output
- 2 additional output giving intermediate results.
- 3 maximum output, showing progress of minimizations.

Note: See also the SET WARnings command.

SET RANdomgenerator <seed>

Sets the seed of the random number generator used in SEEk. This can be any integer between 10 000 and 900 000 000, for example one which was output from a SHOW RANdom command of a previous run.

SET STRategy <level>

Sets the strategy to be used in calculating first and second derivatives and in certain minimization methods. In general, low values of <level> mean fewer function calls and high values mean more reliable minimization. Currently allowed values are 0, 1 (default), and 2.

SET TITLE

Informs Minuit that the next input line is to be considered the (new) title for this task or sub-task. This is for the convenience of the user in reading his output. This command is available only in data-driven mode; in Fortran-callable mode use CALL MNSETI.

SET WARNings

Instructs Minuit to output warning messages when suspicious conditions arise which may indicate unreliable results. This is the default.

SET WIDThpage

Informs Minuit of the output page width. Default values are 80 for interactive jobs and 120 for batch.

SHOw XXXX

All SET XXXX commands have a corresponding SHOw XXXX command. In addition, the SHOw commands listed starting here have no corresponding SET command for obvious reasons. The full list of SHOw commands is printed in response to the command HELP SHOw.

SHOw CORrelations

Calculates and prints the parameter correlations from the error matrix.

SHOw COVariance

Prints the (external) covariance (error) matrix.

SHOw EIGenvalues

Calculates and prints the eigenvalues of the covariance matrix.

SHOw FCNvalue

Prints the current value of FCN.

SIMplex [maxcalls] [tolerance]

Performs a function minimization using the simplex method of Nelder and Mead. Minimization terminates either when the function has been called (approximately) [maxcalls] times, or when the estimated vertical distance to minimum (EDM) is less than [tolerance]. The default value of [tolerance] is $0.1 * UP$ (see SET ERR).

STANDARD

Causes Minuit to execute the Fortran instruction `CALL STAND` where `STAND` is a subroutine supplied by the user.

STOP

Same as `EXIT`.

TOPofpage

Causes Minuit to write the character specified in a `SET PAGETHROW` command (default = 1) to column 1 of the output file, which may or may not position your output medium to the top of a page depending on the device and system. This command can be expected to work properly only for printed output, unfortunately it does not solve the IBM terminal problem.

Chapter 5: How to get the right answer from Minuit.

The goal of Minuit — to be able to minimize and analyze parameter errors for all possible user functions with any number of variable parameters — is of course impossible to realise, even in principle, in a finite amount of time. In practice, some assumptions must be made about the behaviour of the function in order to avoid evaluating it at all possible points. In this chapter we give some hints on how the user can help Minuit to make the right assumptions.

5.1 Which Minimizer to Use.

One of the historically interesting advantages of Minuit is that it was probably the first minimization program to offer the user a choice of several minimization algorithms. This could be taken as a reflection of the fact that none of the algorithms known at that time were good enough to be universal, so users were encouraged to find the one that worked best for them. Since then, algorithms have improved considerably, but Minuit still offers several, mostly so that old users will not feel cheated, but also to help the occasional user who does manage to defeat the best algorithms. Minuit currently offers five commands which can be used to find a smaller function value, in addition to a few others, like MINOS and IMPROVE, which will retain a smaller function value if they stumble on one unexpectedly (or, in the case of IMPROVE, hopefully). The commands which can be used to minimize are:

5.1.1 MIGRAD

This is the best minimizer for nearly all functions. It is a variable-metric method with inexact line search, a stable metric updating scheme, and checks for positive-definiteness. It will run faster if you SET STRATEGY 0 and will be more reliable if you SET STRATEGY 2 (although the latter option may not help much). Its main weakness is that it depends heavily on knowledge of the first derivatives, and fails miserably if they are very inaccurate. If first derivatives are a problem, they can be calculated analytically inside FCN (see elsewhere in this writeup) or if this is not feasible, the user can try to improve the accuracy of Minuit's numerical approximation by adjusting values using the SET EPS and/or SET STRATEGY commands (see Floating Point Precision and SET STRATEGY).

5.1.2 MINIMIZE

This is equivalent to MIGRAD, except that if MIGRAD fails, it reverts to SIMPLEX and then calls MIGRAD again. This is what the old MIGRAD command used to do, but it was removed from the MIGRAD command so that users would have a choice, and because it is seldom of any use to call SIMPLEX when MIGRAD has failed (there are of course exceptions).

5.1.3 SCAN

This is not intended to minimize, and just scans the function, one parameter at a time. It does however retain the best value after each scan, so it does some sort of highly primitive minimization.

5.1.4 SEEK

We have retained this Monte Carlo search mainly for sentimental reasons, even though the limited experience with it is less than spectacular. The method now incorporates a Metropolis algorithm which always moves the search region to be centred at a new minimum, and has probability $e^{(-F/F_{\min})}$ of moving the

search region to a higher point with function value F . This gives it the theoretical ability to jump through function barriers like a multidimensional quantum mechanical tunneler in search of isolated minima, but it is widely believed by at least half of the authors of Minuit that this is unlikely to work in practice (counterexamples are welcome) since it seems to depend critically on choosing the right average step size for the random jumps, and if you knew that, you wouldn't need Minuit.

5.1.5 SIMPLEX

This genuine multidimensional minimization routine is usually much slower than MIGRAD, but it does not use first derivatives, so it should not be so sensitive to the precision of the FCN calculations, and is even rather robust with respect to gross fluctuations in the function value. However, it gives no reliable information about parameter errors, no information whatsoever about parameter correlations, and worst of all cannot be expected to converge accurately to the minimum in a finite time. Its estimate of EDM is largely fantasy, so it would not even know if it did converge.

5.2 Floating point Precision

Minuit figures out at execution time the precision with which it was compiled, and assumes that FCN provides about the same precision. That means not just the length of the numbers used and returned by FCN, but the actual mathematical accuracy of the calculations. The section on Floating point Precision in Chapter One describes what to do if this is not the case.

5.3 Parameter Limits

Putting limits (absolute bounds) on the allowed values for a given parameter, causes Minuit to make a non-linear transformation of its own internal parameter values to obtain the (external) parameter values passed to FCN. To understand the adverse effects of limits, see "The Transformation for Parameters with Limits" in Chapter 1. Basically, the use of limits should be avoided unless needed to keep the parameter inside a desired range.

If parameter limits are needed, in spite of the effects described in Chapter One, then the user should be aware of the following techniques to alleviate problems caused by limits:

5.3.1 Getting the Right Minimum with Limits.

If MIGRAD converges normally to a point where no parameter is near one of its limits, then the existence of limits has probably not prevented Minuit from finding the right minimum. On the other hand, if one or more parameters is near its limit at the minimum, this may be because the true minimum is indeed at a limit, or it may be because the minimizer has become "blocked" at a limit. This may normally happen only if the parameter is so close to a limit (internal value at an odd multiple of $\pm \frac{\pi}{2}$) that Minuit prints a warning to this effect when it prints the parameter values.

The minimizer can become blocked at a limit, because at a limit the derivative seen by the minimizer $\partial F / \partial P_{\text{int}}$ is zero no matter what the real derivative $\partial F / \partial P_{\text{ext}}$ is.

$$\frac{\partial F}{\partial P_{\text{int}}} = \frac{\partial F}{\partial P_{\text{ext}}} \frac{\partial P_{\text{ext}}}{\partial P_{\text{int}}} = \frac{\partial F}{\partial P_{\text{ext}}} = 0$$

For a stepping method (like SIMPLEX) this seldom poses any problem, but a method based on derivatives (MIGRAD) may become blocked at such a value. If this happens, it may be necessary to move the value

of the parameter in question a significant distance from the limit (with `SET PARAM`) and restart the minimization, perhaps with that parameter fixed temporarily. We are investigating ways to induce Minuit to extricate itself from such situations automatically, but it is not so obvious as it seems, and for the moment must sometimes be done by hand.

5.3.2 Getting the right parameter errors with limits.

In the best case, where the minimum is far from any limits, Minuit will correctly transform the error matrix, and the parameter errors it reports should be accurate and very close to those you would have got without limits. In other cases (which should be more common, since otherwise you wouldn't need limits), the very meaning of parameter errors becomes problematic. Mathematically, since the limit is an absolute constraint on the parameter, a parameter at its limit has no error, at least in one direction. The error matrix, which can assign only symmetric errors, then becomes essentially meaningless. On the other hand, the MINOS analysis is still meaningful, at least in principle, as long as MIGRAD (which is called internally by MINOS) does not get blocked at a limit. Unfortunately, the user has no control over this aspect of the MINOS calculation, although it is possible to get enough printout from the MINOS command to be able to determine whether the results are reliable or not.

5.4 Fixing and Releasing Parameters

When Minuit needs to be guided to the “right” minimum, often the best way to do this is with the `FIX` and `RELEASE` commands. That is, suppose you have a problem with ten free parameters, and when you minimize with respect to all at once, Minuit goes to an unphysical solution characterized by an unphysical or unwanted value of parameter number four. One way to avoid this is to `FIX` parameter four at a “good” value (not necessarily the best, since you presumably don't know that yet), and minimize with respect to the others. Then `RELEASE 4` and minimize again. If the problem admits a “good” physical solution, you will normally find it this way. If it doesn't work, you may see what is wrong by the following sequence (where `xxx` is the expected physical value for parameter four):

```
SET PARAM 4 xxx
FIX 4
MIGRAD
RELEASE 4
SCAN 4
```

where the `SCAN` command gives you a picture of `FCN` as a function of parameter four alone, the others being fixed at their current best values. If you suspect the difficulty is due to parameter five, then add the command

```
CONTOUR 4 5
```

to see a two-dimensional picture.

5.5 Interpretation of Parameter Errors

There are two kinds of problems that can arise: The **reliability** of Minuit's error estimates, and their **statistical interpretation**, assuming they are accurate.

5.5.1 Statistical Interpretation.

For discussion of basic concepts, such as the meaning of the elements of the error matrix, parabolic versus MINOS errors, the appropriate value for UP (see SET ERRdef), and setting of exact confidence levels, see (in order of increasing complexity and completeness):

- “*Interpretation of the Errors on Parameters*”, see Part 3 of this write-up.
- “*Determining the Statistical Significance of Experimental Results*”[4].
- “*Statistical Methods in Experimental Physics*”[5].

5.5.2 The Reliability of Minuit Error Estimates.

Minuit always carries around its own current estimates of the parameter errors, which it will print out on request, no matter how accurate they are at any given point in the execution. For example, at initialization, these estimates are just the starting step sizes as specified by the user. After a MIGRAD or HESSE step, the errors are usually quite accurate, unless there has been a problem. Minuit, when it prints out error values, also gives some indication of how reliable it thinks they are. For example, those marked 'CURRENT GUESS ERROR' are only working values not to be believed, and 'APPROXIMATE ERROR' means that they have been calculated but there is reason to believe that they may not be accurate. If no mitigating adjective is given, then at least Minuit believes the errors are accurate, although there is always a small chance that Minuit has been fooled. Some visible signs that Minuit may have been fooled are:

- Warning messages produced during the minimization or error analysis.
- Failure to find new minimum.
- Value of EDM too big. For a “normal” minimization, after MIGRAD, the value of EDM is usually more than three orders of magnitude smaller than UP (the SET ERRordef), unless a looser tolerance has been specified.
- Correlation coefficients exactly equal to zero, unless some parameters are known to be uncorrelated with the others.
- Correlation coefficients very close to one (greater than 0.99). This indicates both an exceptionally difficult problem, and one which has been badly parametrized so that individual errors are not very meaningful because they are so highly correlated.
- Parameter at limit. This condition, signalled by a Minuit warning message, may make both the function minimum and parameter errors unreliable. See section 5.3.2, *Getting the right parameter errors with limits*.

The best way to be absolutely sure of the errors, is to use “independent” calculations and compare them, or compare the calculated errors with a picture of the function if possible. For example, if there is only one free parameter, the command SCAN allows the user to verify approximately the function curvature. Similarly, if there are only two free parameters, use CONTOUR. To verify a full error matrix, compare the results of MIGRAD with those (calculated afterward) by HESSE, which uses a different method. And of course the most reliable and most expensive technique, which must be used if asymmetric errors are required, is MINOS.

5.6 Convergence in MIGRAD, and Positive-definiteness.

MIGRAD uses its current estimate of the covariance matrix of the function to determine the current search direction, since this is the optimal strategy for quadratic functions and “physical” functions should be quadratic in the neighbourhood of the minimum at least. The search directions determined by MIGRAD are guaranteed to be downhill only if the covariance matrix is positive-definite, so in case this is not true, it makes a positive-definite approximation by adding an appropriate constant along the diagonal as determined by the eigenvalues of the matrix. Theoretically, the covariance matrix for a “physical” function must be positive-definite at the minimum, although it may not be so for all points far away from the minimum, even for a well-determined physical problem. Therefore, if MIGRAD reports that it has found a non-positive-definite covariance matrix, this may be a sign of one or more of the following:

- **A non-physical region.** On its way to the minimum, MIGRAD may have traversed a region which has unphysical behaviour, which is of course not a serious problem as long as it recovers and leaves such a region.
- **An underdetermined problem.** If the matrix is not positive-definite even at the minimum, this may mean that the solution is not well-defined, for example that there are more unknowns than there are data points, or that the parametrization of the fit contains a linear dependence. If this is the case, then Minuit (or any other program) cannot solve your problem uniquely, and the error matrix will necessarily be largely meaningless, so the user must remove the underdeterminedness by reformulating the parametrization. Minuit cannot do this itself, but it can provide some hints (contours, global correlation coefficients, eigenvalues) which can help the clever user to find out what is wrong.
- **Numerical inaccuracies.** It is possible that the apparent lack of positive-definiteness is in fact only due to excessive roundoff errors in numerical calculations, either in FCN or in Minuit. This is unlikely in general, but becomes more likely if the number of free parameters is very large, or if the parameters are badly scaled (not all of the same order of magnitude), and correlations are also large. In any case, whether the non-positive-definiteness is real or only numerical is largely irrelevant, since in both cases the error matrix will be unreliable and the minimum suspicious.

5.7 Additional Trouble-shooting

When Minuit just doesn’t work, some of the more common causes are:

- **Precision mismatch.** Make sure your FCN has been compiled with the same precision as the version of Minuit you are using. When using `DOUBLE PRECISION`, it is safest to use the `IMPLICIT` declaration to make sure that everything is `DOUBLE PRECISION`, not just the arguments of FCN but also the internal variables. Note that depending on the computer system used, floating-point constants may be passed as single precision in subroutine arguments, even if there is an `IMPLICIT DOUBLE PRECISION` statement (which is strictly speaking correct since the `IMPLICIT` statement refers only to variables, not constants). Therefore, if constants are used as arguments in subroutine calls, they must be explicitly of the right precision (for example, on Apollo, even `0.` is not equal to `0.DO`).
If the problem is only one of precision, and not of word length mismatch, an appropriate `SET EPS` command may fix it.
- **Trivial bugs in FCN.** The possibilities for Fortran bugs are numerous. Probably the most common among physicists inexperienced in Fortran is the confusion between `REAL` and `INTEGER` types,

which you can sometimes get away with, but not always. [For example, if A and B are REAL variables, the Fortran statement $A = 2*B$ is not good programming, but happens to do what the user probably intended, whereas the statement $A = B + 2/3$ almost certainly will not do what the user intended.] Minuit can spot some trivial bugs itself, and issues a warning when it detects an unusual FCN behaviour. Such a warning should be taken seriously.

Minuit also offers some tools (especially SCAN) which can help the user to find trivial bugs.

- **Overwriting in a user routine.** Overwriting most often occurs when setting the values of a local array or an array in COMMON, and elements outside the dimensions of the array are addressed. Most computer systems do not detect this error unless you attempt to write into a protected area of memory, and of course Minuit is also helpless, especially if Minuit itself is being overwritten. The symptoms of user overwriting may be almost anything, including unusual behaviour of Minuit itself. The effects depend critically on where instructions and data are loaded in memory, so they may change completely if the same program is recompiled with different compiler options or reloaded in a different sequence, even though the compiler and loader are not at fault.
- **Changing the values of input arguments.** In subroutine FCN, for example, the arguments NPAR and IFLAG, as well as the values of the parameters themselves, are only input to FCN and their values should not be changed inside FCN. Minuit is now protected against this in principle, since the user only gets a copy of the value, not the actual address of the internal Minuit variable, but still this is a symptom of misunderstanding by the user.

If you really want to change the number of variable parameters, this must be done with commands like FIX and RELEASE, by redefining parameters using command PARAMETER or CLEAR.

Similarly, if a parameter takes on an unwanted value, it will do no good to change its value inside FCN: In the best case, Minuit won't see your improved value, and in the worst case, it will produce unpredictable results. To set a parameter to a certain value, use the command SET PARam, and to keep it within certain bounds, use the command SET LIMits. If the parameter must obey more complicated constraints, you must find a trick such as adding a penalty value to FCN outside of the physical region, to force it back to where you want it.

- **An ill-posed problem.** For questions of parameter dependence, see the discussion above on positive-definiteness. Other mathematical problems which can arise are: **excessive numerical roundoff** — be especially careful of exponential and factorial functions which get big very quickly and lose accuracy; **starting too far from the solution** — the function may have unphysical local minima, especially at infinity in some variables; **incorrect normalization** — in likelihood functions, the probability distributions must be normalized or at least have an integral which is independent of the values of the variable parameters.
- **A bug in Minuit.** This is extremely unlikely, but it did happen once. If a bug is suspected, and all other possible causes can be eliminated, please try to save a copy of the input and output files, listing of FCN, and other information that may be relevant, and send them to Fred.James@cern.ch.

Chapter 6: A complete example

We give here one full example of a real fit, performed first in batch data-driven mode, then the same fit performed by Fortran calls.

6.1 A data-driven fit

The example job given here is set up for batch processing. The OPEN statements assign the input and output files, and are somewhat computer-dependent (those given here are for a Vax). On many systems, it may be more convenient (or necessary) to perform the file assignments in JCL rather than from the Fortran, but whatever the user decides, the files must be opened and the unit numbers communicated to Minuit before the call to MINUIT.

The same job could be run interactively, in which case the input and output files would be assigned to the terminal, and the “user’s data” listed below, instead of coming from a file, would be typed in directly to the terminal.

The User’s main program

```
PROGRAM DSDQ
EXTERNAL FCNKO
OPEN (UNIT=5,FILE='DSDQ.DAT',STATUS='OLD')
OPEN (UNIT=6,FILE='DSDQ.OUT',STATUS='NEW',FORM='FORMATTED')
CC   CALL MINTIO(5,6,7) ! Not needed, default values
CALL MINUIT(FCNKO,0) ! User routine is called FCNKO
STOP
END
```

The User’s FCN

```
SUBROUTINE FCNKO(NPAR,GIN,F,X,IFLAG,FUTIL)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
REAL THPLUI, THMINI
DIMENSION X(*),GIN(*)
C this subroutine does not use FUTIL
PARAMETER (MXBIN=50)
DIMENSION THPLU(MXBIN),THMIN(MXBIN),T(MXBIN),
+ EVTP(MXBIN),EVTM(MXBIN)
DATA NBINS,NEVTOT/ 30,250/
DATA (EVTP(IGOD),IGOD=1,30)
+ /11., 9., 13., 13., 17., 9., 1., 7., 8., 9.,
+ 6., 4., 6., 3., 7., 4., 7., 3., 8., 4.,
+ 6., 5., 7., 2., 7., 1., 4., 1., 4., 5./
DATA (EVTM(IGOD),IGOD=1,30)
+ / 0., 0., 0., 0., 0., 0., 0., 0., 1., 1.,
+ 0., 2., 1., 4., 4., 2., 4., 2., 2., 0.,
+ 2., 3., 7., 2., 3., 6., 2., 4., 1., 5./
C
XRE = X(1)
XIM = X(2)
DM = X(5)
GAMS = 1.0/X(10)
GAML = 1.0/X(11)
```

```

GAMLS = 0.5*(GAML+GAMS)
IF (IFLAG .NE. 1) GO TO 300
C          generate random data
STHPLU = 0.
STHMIN = 0.
DO 200 I= 1, NBINS
T(I) = 0.1*REAL(I)
TI = T(I)
EHALF = EXP(-TI*GAMLS)
TH = ((1.0-XRE)**2 + XIM**2) * EXP(-TI*GAML)
TH = TH + ((1.0+XRE)**2 + XIM**2) * EXP(-TI*GAMS)
TH = TH - 4.0*XIM*SIN(DM*TI) * EHALF
STERM = 2.0*(1.0-XRE**2-XIM**2)*COS(DM*TI) * EHALF
THPLU(I) = TH + STERM
THMIN(I) = TH - STERM
STHPLU = STHPLU + THPLU(I)
STHMIN = STHMIN + THMIN(I)
200 CONTINUE
NEVPLU = REAL(NEVTOT)*(STHPLU/(STHPLU+STHMIN))
NEVMIN = REAL(NEVTOT)*(STHMIN/(STHPLU+STHMIN))
WRITE (6,'(A)') ' LEPTONIC K ZERO DECAYS'
WRITE (6,'(A,3I10)') ' PLUS, MINUS, TOTAL=',NEVPLU,NEVMIN,NEVTOT
WRITE (6,'(A)')
+ '0 TIME THEOR+ EXPTL+ THEOR- EXPTL-'
SEVTP = 0.
SEVTM = 0.
DO 250 I= 1, NBINS
THPLU(I) = THPLU(I)*REAL(NEVPLU) / STHPLU
THMIN(I) = THMIN(I)*REAL(NEVMIN) / STHMIN
THPLUI = THPLU(I)
CCCCC      remove the CCC to generate random data
CCC      CALL POISSN(THPLUI,NP,IERROR)
CCC      EVTP(I) = NP
SEVTP = SEVTP + EVTP(I)
THMINI = THMIN(I)
CCC      CALL POISSN(THMINI,NM,IERROR)
CCC      EVTM(I) = NM
SEVTM = SEVTM + EVTM(I)
IF (IFLAG .NE. 4)
+ WRITE (6,'(1X,5G12.4)') T(I),THPLU(I),EVTP(I),THMIN(I),EVTM(I)
250 CONTINUE
WRITE (6,'(A,2F10.2)') ' DATA EVTS PLUS, MINUS=', SEVTP,SEVTM
C          calculate chisquare
300 CONTINUE
CHISQ = 0.
STHPLU = 0.
STHMIN = 0.
DO 400 I= 1, NBINS
TI = T(I)
EHALF = EXP(-TI*GAMLS)
TH = ((1.0-XRE)**2 + XIM**2) * EXP(-TI*GAML)
TH = TH + ((1.0+XRE)**2 + XIM**2) * EXP(-TI*GAMS)
TH = TH - 4.0*XIM*SIN(DM*TI) * EHALF
STERM = 2.0*(1.0-XRE**2-XIM**2)*COS(DM*TI) * EHALF
THPLU(I) = TH + STERM
THMIN(I) = TH - STERM
STHPLU = STHPLU + THPLU(I)

```

```

      STHMIN = STHMIN + THMIN(I)
400 CONTINUE
      THP = 0.
      THM = 0.
      EVP = 0.
      EVM = 0.
      IF (IFLAG .NE. 4) WRITE (6,'(1H0,10X,A,20X,A)')
+ 'POSITIVE LEPTONS','NEGATIVE LEPTONS'
      IF (IFLAG .NE. 4) WRITE (6,'(A,3X,A)')
+ '      TIME      THEOR      EXPTL      CHISQ',
+ '      TIME      THEOR      EXPTL      CHISQ'
C
      DO 450 I= 1, NBINS
      THPLU(I) = THPLU(I)*SEVTP / STHPLU
      THMIN(I) = THMIN(I)*SEVTM / STHMIN
      THP = THP + THPLU(I)
      THM = THM + THMIN(I)
      EVP = EVP + EVTP(I)
      EVM = EVM + EVTM(I)
C Sum over bins until at least four events found
      IF (EVP .GT. 3.) THEN
          CHI1 = (EVP-THP)**2/EVP
          CHISQ = CHISQ + CHI1
          IF (IFLAG .NE. 4)
+           WRITE (6,'(1X,4F9.3)') T(I),THP,EVP,CHI1
          THP = 0.
          EVP = 0.
      ENDIF
      IF (EVM .GT. 3) THEN
          CHI2 = (EVM-THM)**2/EVM
          CHISQ = CHISQ + CHI2
          IF (IFLAG .NE. 4)
+           WRITE (6,'(42X,4F9.3)') T(I),THM,EVM,CHI2
          THM = 0.
          EVM = 0.
      ENDIF
450 CONTINUE
      F = CHISQ
      RETURN
      END

```

The user's data to drive Minuit.

```

set title
FIT DELTA S/ DELTA Q RULE TO LEPTONIC K ZERO DECAYS
parameters
1 'Real(X)' 0. .1
2 'Imag(X)' 0. .1
5 'Delta M' .535 .01
10 'K Short LT' .892
11 'K Long LT' 518.3

fix 5
migr
print 0
set print 0
minos

```



```

restore
migrad
minos
set param 5 0.535
fix 5
contour 1 2
stop

```

6.2 The same example in Fortran-callable mode.

The program below takes the place of the data in the above example.

The User's main program and subroutine

```

PROGRAM DSDQ
C      Minit test case. Fortran-callable.
C      Fit randomly-generated leptonic K0 decays to the
C      time distribution expected for interfering K1 and K2,
C      with free parameters Re(X), Im(X), DeltaM, and GammaS.
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
EXTERNAL FCNKO
CC OPEN (UNIT=6,FILE='DSDQ.OUT',STATUS='NEW',FORM='FORMATTED')
DIMENSION NPRM(5),VSTRT(5),STP(5),ARGLIS(10)
CHARACTER*10 PNAM(5)
DATA NPRM / 1 , 2 , 5 , 10 , 11 /
DATA PNAM / 'Re(X)', 'Im(X)', 'Delta M', 'T Kshort', 'T Klong' /
DATA VSTRT/ 0. , 0. , .535 , .892 , 518.3 /
DATA STP / 0.1 , 0.1 , 0.1 , 0. , 0. /
C      Initialize Minit, define I/O unit numbers
CALL MNINIT(5,6,7)
C      Define parameters, set initial values
ZERO = 0.
DO 11 I= 1, 5
CALL MNPARM(NPRM(I),PNAM(I),VSTRT(I),STP(I),ZERO,ZERO,IERFLG)
IF (IERFLG .NE. 0) THEN
WRITE (6,'(A,I)') ' UNABLE TO DEFINE PARAMETER NO.',I
STOP
ENDIF
11 CONTINUE
C
CALL MNSETI('Time Distribution of Leptonic K0 Decays')
C      Request FCN to read in (or generate random) data (IFLAG=1)
ARGLIS(1) = 1.
CALL MNEXCM(FCNKO, 'CALL FCN', ARGLIS ,1,IERFLG)
C
ARGLIS(1) = 5.
CALL MNEXCM(FCNKO,'FIX', ARGLIS ,1,IERFLG)
ARGLIS(1) = 0.
CALL MNEXCM(FCNKO,'SET PRINT', ARGLIS ,1,IERFLG)
CALL MNEXCM(FCNKO,'MIGRAD', ARGLIS ,0,IERFLG)
CALL MNEXCM(FCNKO,'MINOS', ARGLIS ,0,IERFLG)
CALL PRERR
ARGLIS(1) = 5.
CALL MNEXCM(FCNKO,'RELEASE', ARGLIS ,1,IERFLG)
CALL MNEXCM(FCNKO,'MIGRAD', ARGLIS ,0,IERFLG)
CALL MNEXCM(FCNKO,'MINOS', ARGLIS ,0,IERFLG)

```

```
      ARGLIS(1) = 3.
      CALL MNEXCM(FCNKO,'CALL FCN', ARGLIS , 1,IERFLG)
      CALL PRERR
      CALL MNEXCM(FCNKO,'STOP ', 0,0,IERFLG)
      STOP
      END

      SUBROUTINE PRERR
C   a little hand-made routine to print out parameter errors
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C   find out how many variable parameters there are
      CALL MNSTAT(FMIN,FEDM,ERRDEF,NPARI,NPARX,ISTAT)
C   and their errors
      DO 50 I= 1, NPARI
      CALL MNERRS(-I,EPLUS,EMINUS,EPARAB,GLOBCC)
      WRITE (6,45) I,EPLUS,EMINUS,EPARAB,GLOBCC
45  FORMAT (5X,I5,4F12.6)
50  CONTINUE
      RETURN
      END
```

The FCN is exactly the same in Fortran-callable mode as in data-driven mode.

Chapter 7: Interpretation of the errors on Minit parameters

It often happens that the solution of a minimization problem using Minit is itself straightforward, but the calculation or interpretation of the resulting parameter uncertainties is considerably more complicated. The purpose of this chapter is to clarify the most commonly encountered difficulties in parameter error determination. These difficulties may arise in connection with any fitting program, are discussed here with Minit terminology.

The most common causes of misinterpretation may be grouped into three categories:

- 1 Proper normalization of the user-supplied chi-square or likelihood function, and appropriate ERROR DEF.
- 2 Non-linearities in the problem formulation, leading to different errors being calculated by different techniques, such as MIGRAD, HESSE and MINOS.
- 3 Multiparameter error definition and interpretation.

All these topics are discussed in some detail in Eadie et al.[5], which may be consulted for further details.

7.1 Function normalization and ERROR DEF

In order to provide for full generality in the user-defined function value, the user is allowed to define a normalization factor known internally as UP and defined by the Minit user on an ERROR DEF command card. The default value is one. The Minit error on a parameter is defined as the change of parameter which would produce a change of the function value equal to UP. This is the most general way to define the error, although in statistics it is more usual to define it in terms of the second derivative of the χ^2 function – with respect to the parameter in question. In the simplest linear case (when the function is exactly parabolic at the minimum), the value UP=1.0 corresponds to defining the error as the inverse of the second derivative at the minimum. The fact that Minit defines the error in terms of a function change does not mean that it always calculates such a function change. Indeed it sometimes (HESSE) calculates the second derivative matrix and inverts it, assuming a parabolic behaviour. This distinction is discussed in section 7.2.

The purpose of defining errors by function changes is threefold:

- 1 to preserve its meaning in the non-parabolic case (see section 7.2);
- 2 to allow generality when the user-defined function is not a chi-square or likelihood, but has some other origin;
- 3 to allow calculation not only of “one-standard deviation” errors, but also two or more standard deviations, or more general ‘confidence regions’, especially in the multiparameter case (see section 7.3).

7.1.1 Chi-square normalization

If the user’s function value F is supposed to be a chisquare, it must of course be properly normalized. That is, the “weights” must in fact correspond to the one-standard-deviation errors on the observations. The most general expression for the chi-square χ is of the form (see [5], p.163):

$$\chi^2 = \sum_{i,j} (x_i - y_i(a)) V_{ij} (x_j - y_j(a))$$

where x is the vector of observations, $y(a)$ is the vector of fitted values (or theoretical expressions for them) containing the variable fit parameters a , and V is the inverse of the error matrix of the observations x , also known as the covariance matrix of the observations.

Fortunately, in most real cases the observations x are statistically independent of each other (e.g., the contents of the bins of a histogram, or measurements of points on a trajectory), so the matrix V is diagonal only. The expression for χ^2 then simplifies to the more familiar form:

$$\chi^2 = \sum_i \frac{(x_i - y_i(a))^2}{e_i^2}$$

where e^2 is the inverse of the diagonal element of V , the square of the error on the corresponding observation x . In the case where the x are integer numbers of events in an unweighted histogram, for example, the e^2 are just equal to the x (or to the y , see [5], pp.170-171).

The minimization of χ^2 above is sometimes called **weighted least squares** in which case the inverse quantities $1/e^2$ are called the weights. Clearly this is simply a different word for the same thing, but in practice the use of these words sometimes means that the interpretation of e^2 as variances or squared errors is not straightforward. The word weight often implies that only the relative weights are known (“point two is twice as important as point one”) in which case there is apparently an unknown overall normalization factor. Unfortunately the parameter errors coming out of such a fit will be proportional to this factor, and the user must be aware of this in the formulation of his problem.

The e^2 may also be functions of the fit parameters a (see [5], pp.170-171). Normally this results in somewhat slower convergence of the fit since it usually increases the nonlinearity of the fit. (In the simplest case it turns a linear problem into a non-linear one.) However, the effect on the fitted parameter values and errors should be small.

If the user’s chi-square function is correctly normalized, he should use UP=1.0 (the default value) to get the usual one standard-deviation errors for the parameters one by one. To get two-standard-deviation errors, use ERROR DEF 4.0, etc., since the chisquare dependance on parameters is quadratic. For more general confidence regions involving more than one parameter, see section 7.2.

7.1.2 Likelihood normalization

If the user function is a negative log-likelihood function, it must again be correctly normalized, but the reasons and ensuing problems in this case are quite different from the chisquare case. The likelihood function takes the form (see [5], p. 155):

$$F = - \sum_i \ln f(x_i, a)$$

where each x represents in general a vector of observations, the a are the free parameters of the fit, and the function f represents the hypothesis to be fitted. This function f must be normalized:

$$\int f(x_i, a) dx_1 dx_2 \dots dx_n = \text{constant}$$

that is, the integral of f over all observation space x must be independent of the fit parameters a .

The consequence of not normalizing f properly is usually that the fit simply will not converge, some parameters running away to infinity. Strangely enough, the value of the normalization constant does

not affect the fitted parameter values or errors, as can be seen by the fact that the logarithm makes a multiplicative constant into an additive one, which simply shifts the whole log-likelihood curve and affects its value, but not the fitted parameter values or errors. In fact, the actual value of the likelihood at the minimum is quite meaningless (unlike the chi-square value) and even depends on the units in which the observation space x is expressed. The meaningful quantity is the difference in log-likelihood between two points in parameter-space, which is dimensionless.

For likelihood fits, the value $UP=0.5$ corresponds to one-standard-deviation errors. Or, alternatively, F may be defined as $-2 \log(\text{likelihood})$, in which case differences in F have the same meaning as for chi-square and $UP=1.0$ is appropriate. The two different ways of introducing the factor of 2 are quite equivalent in Minuit, and although most people seem to use $UP=0.5$, it is perhaps more logical to put the factor 2 directly into FCN.

7.2 Non-linearities: MIGRAD versus HESSE versus MINOS

In the theory of statistics, one can show that in the asymptotic limit, any of several methods of determining parameter errors are equivalent and will give the same result. Let us for the moment call these methods MIGRAD, HESSE, and MINOS (SIMPLEX is a special case). It turns out that the conditions under which these methods yield exactly the same errors are either of the following:

- 1 The model to be fitted (y or f) is exactly a linear function of the fit parameters a , or
- 2 The amount of observed data is infinite.

It may happen that (1) is satisfied, in which case you don't really need Minuit, a smaller, simpler, and faster program would do, since a linear problem can be solved directly without iterations (see [5], p. 163-165), for example with CERN library program LSQQR. Nevertheless, it may be convenient to use Minuit since non-linear terms can then be added later if desired, without major changes to the method. Condition (2) is of course never satisfied, although in practice it often happens that there is enough data to make the problem "almost linear", that is there is so much data that the range of parameters allowed by the data becomes very small, and any physical function behaves linearly over a small enough region. The following sections explain the differences between the various parameter errors given by Minuit.

7.2.1 Errors printed by Minuit

The errors printed by Minuit at any given stage represent the best symmetric error estimates available at that stage, which may not be very good. For example, at the first entry to FCN, the user's step sizes are given, and these may bear no resemblance at all to proper parameter errors, although they are supposed to be order-of-magnitude estimates. After crude minimizers like SEEK or SIMPLEX, a revised error estimate may be given, but this too is only meant to be an order-of-magnitude estimate, and must certainly not be taken seriously as a physical result. Such numbers are mainly for the internal use of Minuit, which must after all assume a step size for future minimizations and derivative calculations, and uses these "errors" as a first guess to be modified on the basis of experience.

7.2.2 Errors after MIGRAD (or MINIMIZE)

The minimizing technique currently implemented in MIGRAD is a stable variation (the "switching" method) of the Davidon-Fletcher-Powell variable-metric algorithm. This algorithm converges to the correct error matrix as it converges to the function minimum.

This algorithm requires at each step a “working approximation” of the error matrix, and a rather good approximation to the gradient vector at the current best point. The starting approximation to the error matrix may be obtained in different ways, depending on the status of the error matrix before MIGRAD is called as well as the value of STRATEGY. Usually it is found to be advantageous to evaluate the error matrix rather carefully at the start point in order to avoid premature convergence, but in principle even the unit matrix can be used as a starting approximation. Usually the Minuit default is to start by calculating the full error matrix by calculating all the second derivatives and inverting the matrix. If the user wants to make sure this is done, he can call HESSE before MIGRAD.

If a unit matrix is taken to start, then the first step will be in a *steepest descent* direction, which is not bad, but the estimate of EDM, needed to judge convergence, will be poor. At each successive step, the information gathered from the change of gradient is used to improve the approximation to the error matrix, without the need to calculate any second derivatives or invert any matrices. The algorithm used for this *updating* is supposed to be the best known, but if there are a lot of highly correlated parameters, it may take many steps before the off-diagonal elements of the error matrix approach the correct values. In practice, MIGRAD usually yields good estimates of the error matrix, but it is not absolutely reliable for two reasons:

- 1 Convergence to the minimum may occur “too fast” for MIGRAD to have a good estimate of the error matrix. In the most flagrant of such cases, MIGRAD realizes this and automatically introduces an additional call to HESSE (described below), informing the user that the covariance matrix is being recalculated. Since, for n variable parameters, there are $n(n + 1)/2$ elements in the error matrix, the number of FCN calls from MIGRAD must be large compared with n^2 in order for the MIGRAD error matrix calculation to be reliable.
- 2 MIGRAD gathers information about the error matrix as it proceeds, based on function values calculated away from the minimum and assuming that the error matrix is nearly constant as a function of the parameters, as it would be if the problem were nearly linear. If the problem is highly non-linear, the error matrix will depend strongly on the parameters, MIGRAD will converge more slowly, and the resulting error matrix will at best represent some average over the last part of the trajectory in parameter-space traversed by MIGRAD.

If MIGRAD errors are wrong because of (1), HESSE should be commanded after MIGRAD and will give the correct errors. If MIGRAD errors are wrong because of (2), HESSE will help, but only in an academic sense, since in this case the error matrix is not the whole story and for proper error calculation MINOS must be used.

As a general rule, anyone seriously interested in the parameter errors should always put at least a HESSE command after each MIGRAD (or MINIMIZE) command.

7.2.3 Errors after HESSE

HESSE simply calculates the full second-derivative matrix by finite differences and inverts it. It therefore calculates the error matrix at the point where it happens to be when it is called. If the error matrix is not positive-definite, diagnostics are printed, and an attempt is made to form a positive-definite approximation. The error matrix must be positive-definite at the solution (minimum) for any real physical problem. It may well not be positive away from the minimum, but most algorithms including the MIGRAD algorithm require a positive-definite “working matrix”.

The error matrix produced by HESSE is used to calculate what Minuit prints as the parameter errors, which therefore contain the effects due to parameter correlations. The extent of the two-by-two correlations can

be seen from the correlation coefficients printed by Minuit, and the global correlations (see [5], p. 23) are also printed. All of these correlation coefficients must be less than one in absolute value. If any of them are very close to one or minus one, this indicates an illposed problem with more free parameters than can be determined by the model and the data.

7.2.4 Errors by MINOS

MINOS is designed to calculate the correct errors in all cases, especially when there are non-linearities as described above. The theory behind the method is described in [5], pp. 204-205 (where “non-parabolic likelihood” should of course read “non-parabolic log-likelihood”, which is equivalent to “nonparabolic chi-square”).

MINOS actually follows the function out from the minimum to find where it crosses the function value (minimum + UP), instead of using the curvature at the minimum and assuming a parabolic shape. This method not only yields errors which may be different from those of HESSE, but in general also different positive and negative errors (asymmetric error interval). Indeed the most frequent result for most physical problems is that the (symmetric) HESSE error lies between the positive and negative errors of MINOS. The difference between these three numbers is one measure of the non-linearity of the problem (or rather of its formulation).

In practice, MINOS errors usually turn out to be close to, or somewhat larger than errors derived from the error matrix, although in cases of very bad behaviour (very little data or ill-posed model) anything can happen. In particular, it is often not true in MINOS that two-standard-deviation errors (UP=4) and three-standard-deviation errors (UP=9) are respectively two and three times as big as one-standard-deviation errors, as is true by definition for errors derived from the error matrix (MIGRAD or HESSE).

7.3 Multiparameter errors

In addition to the difficulties described above, a special class of problems arise in interpreting errors when there is more than one free parameter. These problems are quite separate from those described above and are really much simpler in principle, although in practice confusion often arises.

7.3.1 The Error Matrix

The error matrix, also called the covariance matrix, is the inverse of the second derivative matrix of the (log-likelihood or chisquare) function with respect to its free parameters, usually assumed to be evaluated at the best parameter values (the function minimum). The diagonal elements of the error matrix are the squares of the individual parameter errors, **including the effects of correlations** with the other parameters.

The inverse of the error matrix, the second derivative matrix, has as diagonal elements the second partial derivatives with respect to one parameter at a time. These diagonal elements are not therefore coupled to any other parameters, but when the matrix is inverted, the diagonal elements of the inverse contain contributions from all the elements of the second derivative matrix, which is “where the correlations come from”.

Although a parameter may be either positively or negatively correlated with another, the effect of correlations is always to increase the errors on the other parameters in the sense that if a given free parameter suddenly became exactly known (fixed), that would always decrease (or at least not change) the errors on the other parameters. In order to see this effect quantitatively, the following procedure can be used to “delete” one parameter from the error matrix, including its effects on the other parameters:

- 1 Invert the error matrix, to yield the second-derivative matrix.
- 2 Remove the row and column of the inverse corresponding to the given parameter.
- 3 Re-invert the resulting (smaller) matrix.

This reduced error matrix will have its diagonal elements smaller or equal to the corresponding elements in the original error matrix, the difference representing the effect of knowing or not knowing the true value of the parameter that was removed at step two. This procedure is exactly that performed by Minuit when a FIX command is executed. Note that it is not reversible, since information has been lost in the deletion. The Minuit commands RESTORE and RELEASE therefore cause the error matrix to be considered lost and it must be recalculated entirely.

7.3.2 MINOS with several free Parameters

The MINOS algorithm is described in some detail in part 1 of this manual. Here we add some supplementary “geometrical interpretation” for the multidimensional case.

Let us consider that there are just two free parameters, and draw the contour line connecting all points where the function takes on the value $F_{\min} + \text{UP}$. (The CONTOUR command will do this for you from Minuit). For a linear problem, this contour line would be an exact ellipse, the shape and orientation of which are described in [5], p.196 (Fig. 9.4). For our problem let the contour be as in figure 7.1. If MINOS is requested to find the errors in parameter one (the x-axis), it will find the extreme contour points A and B, whose x-coordinates, relative to the x-coordinate at the minimum (X), will be respectively the negative and positive MINOS errors of parameter one.

7.3.3 Probability content of confidence regions

For an n -parameter problem MINOS performs minimizations in $(n - 1)$ dimensions in order to find the extreme points of the hypercontour of which a two-dimensional example is given in figure 7.1, and in this way takes account of all the correlations with the other $n - 1$ parameters. However, the errors which it calculates are still only single-parameter errors, in the sense that each parameter error is a statement only about the value of that parameter. This is represented geometrically by saying that the confidence region expressed by the MINOS error in parameter one is the grey area of figure 7.2, extending to infinity at both the top and bottom of the figure.

If UP is set to the appropriate one-standard-deviation value, then the precise meaning of the confidence region of figure 7.2 is: “The probability that the true value of parameter one lies between A and B is 68.3%” (the probability of a normally-distributed parameter lying within one std.-dev. of its mean). That is, the probability content of the grey area in figure 7.2 is 68.3%. No statement is made about the simultaneous values of the other parameter(s), since the grey area covers all values of the other parameter(s).

If it is desired to make **simultaneously** statements about the values of two or more parameters, the situation becomes considerably more complicated and the probabilities get much smaller. The first problem is that of choosing the shape of the confidence region, since it is no longer simply an interval on an axis, but a hypervolume. The easiest shape to express is the hyperrectangle given by:

$$\begin{aligned} A < \text{param 1} < B \\ C < \text{param 2} < D \\ E < \text{param 3} < F, \text{ etc.} \end{aligned}$$

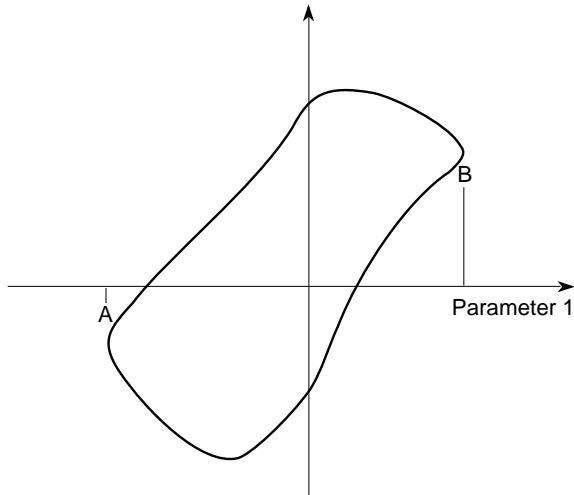


Figure 7.1: MINOS errors for parameter 1

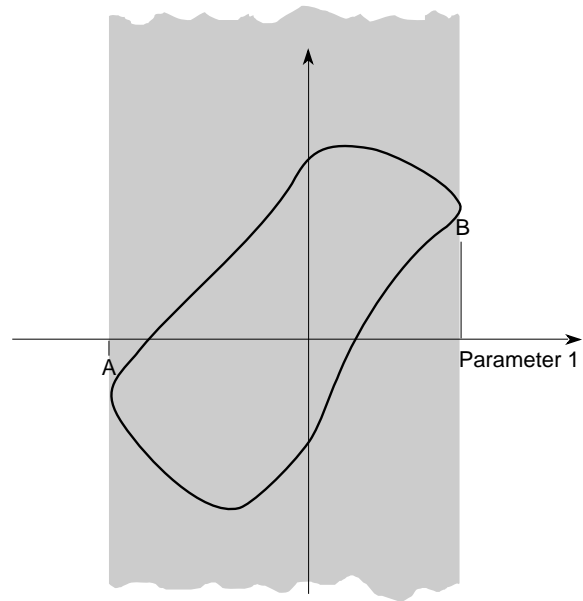


Figure 7.2: MINOS error confidence region for parameter 1

This confidence region for our two-parameter example is the grey area in figure 7.3. However, there are two good reasons not to use such a shape:

1. Some regions inside the hyperrectangle (namely the corners) have low likelihoods, lower than some regions just outside the rectangle, so the hyperrectangle is not the optimal shape (does not contain the most likely points).
2. One does not know an easy way to calculate the probability content of these hyperrectangles (see [5], p.196-197, especially fig. 9.5a).

For these reasons one usually chooses regions delimited by contours of equal likelihood (hyperellipsoids in the linear case). For our two-parameter example, such a confidence region would be the grey region in figure 7.4, and the corresponding probability statement is: “The probability that parameter one and parameter two simultaneously take on values within the one-standard-deviation likelihood contour is 39.3%”.

The probability content of confidence regions like those shaded in figure 7.4 becomes very small as the number of parameters N_{PAR} increases, for a given value of UP . Such probability contents are in fact the probabilities of exceeding the value UP for a chisquare function of N_{PAR} degrees of freedom, and can therefore be read off from tables of chisquare. Table 7.1 gives the values of UP which yield hypercontours enclosing given probability contents for given number of parameters.

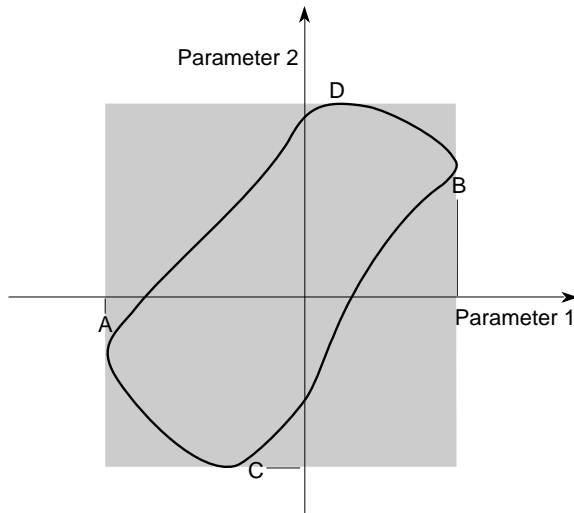


Figure 7.3: Rectangular confidence region for parameters 1 and 2

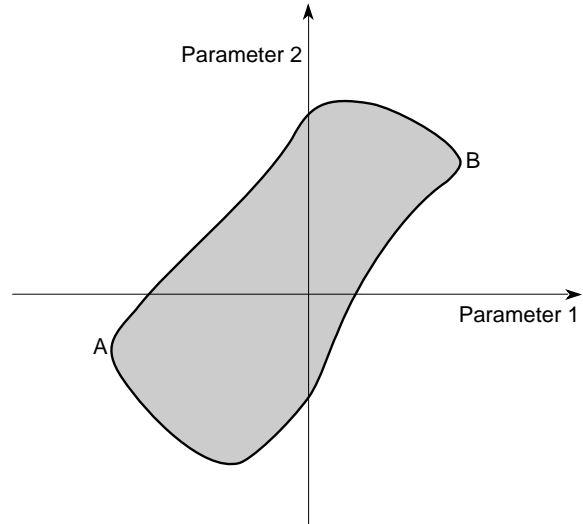


Figure 7.4: Optimal confidence region for parameters 1 and 2

Number of Parameters	Confidence level (probability contents desired inside hypercontour of $\chi^2 = \chi_{\min}^2 + \text{UP}$)				
	50%	70%	90%	95%	99%
1	0.46	1.07	2.70	3.84	6.63
2	1.39	2.41	4.61	5.99	9.21
3	2.37	3.67	6.25	7.82	11.36
4	3.36	4.88	7.78	9.49	13.28
5	4.35	6.06	9.24	11.07	15.09
6	5.35	7.23	10.65	12.59	16.81
7	6.35	8.38	12.02	14.07	18.49
8	7.34	9.52	13.36	15.51	20.09
9	8.34	10.66	14.68	16.92	21.67
10	9.34	11.78	15.99	18.31	23.21
11	10.34	12.88	17.29	19.68	24.71
If FCN is $-\log(\text{likelihood})$ instead of χ^2 , all values of UP should be divided by 2.					

Table 7.1: Table of UP for multi-parameter confidence regions

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