An Introduction to

AD MODEL BUILDER

for Use in Nonlinear Modeling and Statistics

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`http://admb-project.org/documentation/manuals`

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Chapter 1

Getting Started with AD Model Builder

This manual describes AD Model Builder, the fastest, most powerful software for rapid development and fitting of general nonlinear statistical models available. The accompanying demonstration disk has a number of example programs from various fields, including chemical engineering, natural resource modeling, and financial modeling. As you will see, with a few statements, you can build powerful programs to solve problems that would completely defeat other modeling environments. The AD Model Builder environment makes it simple to deal with recurring difficulties in nonlinear modeling, such as restricting the values that parameters can assume, carrying out the optimization in a stepwise manner, and producing a report of the estimates of the standard deviations of the parameter estimates. In addition, these techniques scale up to models with at least 5000 independent parameters on a basic laptop, and more on more powerful platforms. So, if you are interested in a really powerful environment for nonlinear modeling—read on!

AD Model Builder provides a template-like approach to code generation. Instead of needing to write all the code for the model, the user can employ any ASCII file editor to simply fill in the template, describing the particular aspects of the model—data, model parameters, and the fitting criterion—to be used. With this approach, the specification of the model is reduced to the absolute minimum number of statements. Reasonable default behavior for various aspects of modeling, such as the input of data and initial parameters, and reporting of results, are provided. Of course, it is possible to override this default behavior to customize an application when desired. The command line argument `-ind NAME` followed by the string `NAME` changes the default data input file to `NAME`, where `NAME` is any name you like.

The various concepts embodied in AD Model Builder are introduced in a series of examples. You should at least skim through each of the examples in the order they appear, so that you will be familiar with the concepts used in the later examples. The examples disk contains the AD Model Builder template code, the C++ code produced by AD Model Builder, and the executable programs produced by compiling the C++ code. This process of producing the executable is automated, so that the user who doesn't wish to consider the vagaries of C++ programming can go from the AD Model Builder template to the compiled executable in one step. Assuming that the C++ compiler and the AD Model Builder

and AUTODIF libraries have been properly installed, then to produce a AD Model Builder executable, it is only necessary to type `makeadm root`, where `root.tpl` is the name of the ASCII file containing the template specification. To simplify model development, two modes of operation are provided: a safe mode with bounds checking on all array objects, and an optimized mode, for fastest execution.

AD Model Builder achieves its high performance levels by employing the AUTODIF C++ class library. AUTODIF combines an array language with the reverse mode of automatic differentiation, supplemented with precompiled adjoint code for the derivatives of common array and matrix operations. However, all of this is completely transparent to the AD Model Builder user. It is only necessary to provide a simple description of the statistical model desired, and the entire process of fitting the model to data and reporting the results is taken care of automatically.

Although C++ potentially provides good support for mathematical modeling, the language is rather complex—it cannot be learned in a few days. Moreover, many features of the language are not needed for mathematical modeling. A novice user who wishes to build mathematical models may have a difficult time deciding what features of the language to learn and what features can be ignored until later. AD Model Builder is intended to help overcome these difficulties and to speed up model development. When using AD Model Builder, most of the aspects of C++ programming are hidden from the user. In fact, the beginning user can be almost unaware that C++ underlies the implementation of AD Model Builder. It is only necessary to be familiar with some of the simpler aspects of C or C++ syntax.

To interpret the results of the statistical analysis, AD Model Builder provides simple methods for calculating the profile likelihood and Markov chain simulation estimates of the posterior distribution for parameters of interest (Hastings-Metropolis algorithm).

1.1 What are nonlinear statistical models?

AD Model Builder is software for creating computer programs to estimate the parameters (or the probability distribution of parameters) for nonlinear statistical models. This raises the question: "What is a nonlinear statistical model?" Consider the following model. We have a set of observations Y_i and x_{ij}, where it is assumed that

$$Y_i = \sum_{j=1}^{m} a_j x_{ij} + \epsilon_i, \tag{1.1}$$

and where the ϵ_i are assumed to be normally distributed random variables with equal variance σ^2. Given these assumptions, it can be shown that "good" estimates for the unknown parameters a_j are obtained by minimizing

$$\sum_i \left(Y_i - \sum_{j=1}^{m} a_j x_{ij} \right)^2 \tag{1.2}$$

with respect to these parameters. These minimizing values can be found by taking the derivatives with respect to the a_j and setting them equal to zero. Since equation (1.1) is linear in the a_j and equation (1.2) is quadratic, it follows that the equations given by setting the derivatives equal to zero are linear in the a_j. So, the estimates can be found by solving a system of linear equations. For this reason, such a statistical model is referred to as "linear." Over time, very good numerically stable methods have been developed for calculating these least-squares estimates. For situations where either the equations in the model corresponding to equation (1.1) are not linear, or the statistical assumptions involve non-normal random variables, the methods for finding good parameter estimates will involve minimizing functions that are not quadratic in the unknown parameters a_j.

In general, these optimization problems are much more difficult than those arising in least-squares problems. There are, however, various techniques that render the estimation of parameters in such nonlinear models more tractable. The AD Model Builder package is intended to organize these techniques in such a way that they are easy to employ (where possible, employing them in a way that the user does not need to be aware of them), so that investigating nonlinear statistical models becomes—so far as possible—as simple as for linear statistical models.

1.2 Installing the software

AD Model Builder is available without charge from http://admb-project.org/downloads/. Libraries compiled for most common combinations of computer architectures, operating systems, and compilers (including Windows, Linux, MacOS and OpenSolaris) and the complete source code are available.

Installation instructions for different compilers are also available on-line at
http://admb-project.org/documentation/installation

1.3 The sections in an AD Model Builder TPL file

An AD Model Builder template (TPL file) consists of up to 11 sections. Eight of these sections are optional. Optional sections are enclosed in brackets [ ]. The optional `FUNCTION` keyword defines a subsection of the `PROCEDURE_SECTION`.

The simplest model contains only the three required sections:

- a `DATA_SECTION`,
- a `PARAMETER_SECTION`, and
- a `PROCEDURE_SECTION`.

For example,

```
DATA_SECTION

[INITIALIZATION_SECTION]

PARAMETER_SECTION

[PRELIMINARY_CALCS_SECTION]

PROCEDURE_SECTION
  [FUNCTION]

[REPORT_SECTION]

[RUNTIME_SECTION]

[TOP_OF_MAIN_SECTION]

[GLOBALS_SECTION]

[BETWEEN_PHASES_SECTION]

[FINAL_SECTION]
```

1.4 The original AD Model Builder examples

This section includes a short description of the original examples distributed with AD Model Builder. There are now many more examples, which are discussed in subsequent chapters.

A very simple example. This is a trivial least-squares linear model, which is included simply to introduce the basics of AD Model Builder.

A simple nonlinear regression model for estimating the parameters describing a von Bertalanffy growth curve from size-at-age data. AD Model Builder's robust regression routine is introduced and used to illustrate how problems caused by "outliers" in the data can be avoided.

A chemical kinetics problem. A model defined by a system of ordinary differential equations. The purpose is to estimate the parameters that describe the chemical reaction.

A problem in financial modeling. A Generalized Autoregressive Conditional Heteroskedasticity, or GARCH, model is used to attempt describing the time series of returns from

some market instrument.

A problem in natural resource management. The Schaefer-Pella-Tomlinson Model for investigating the response of an exploited fish population is developed and extended to include a Bayesian times series treatment of time-varying carrying capacity. This example is interesting because the model is rather temperamental. Several techniques for producing reliable convergence of the estimation procedure to the correct answer are described. For one of the data sets, over 100 parameters are estimated.

A simple fisheries catch-at-age model. These models are used to try and estimate the exploitation rates, etc., in exploited fish populations.

More complex examples are presented in subsequent chapters.

1.5 Example 1: linear least squares

To illustrate this method, we begin with a simple statistical model, which is to estimate the parameters of a linear relationship of the form

$$Y_i = ax_i + b \qquad \text{for } 1 <= i <= n,$$

where x_i and Y_i are vectors, and a and b are the model parameters that are to be estimated. The parameters are estimated by the method of least squares—that is, we find the values of a and b such that the sum of the squared differences between the observed values Y_i and the predicted values $ax_i + b$ is minimized. That is, we want to solve the problem

$$\min_{a,b} \sum_{i=1}^{n} (Y_i - ax_i - b)^2$$

The template for this model is in the file `SIMPLE.TPL`. To make the model, one would type `makeadm simple`. The resulting executable for the model is in the file `SIMPLE.EXE`. The contents of `SIMPLE.TPL` are below. (Anything following "`//`" is a comment.)

```
DATA_SECTION
  init_int nobs           // nobs is the number of observations
  init_vector Y(1,nobs)   // the observed Y values
  init_vector x(1,nobs)
PARAMETER_SECTION
  init_number a
  init_number b
  vector pred_Y(1,nobs)
  objective_function_value f
PROCEDURE_SECTION
```

```
  pred_Y=a*x+b;      // calculate the predicted Y values
  f=regression(Y,pred_Y); // do the regression---the vector of
                          // observations goes first
```

The main requirement is that all keywords must begin in column 1, while the code itself must be indented.

1.6 The data section

Roughly speaking, the data consist of the stuff in the real world that you observe and want to analyze. The data section describes the structure of the data in your model. Data objects consist of integers (`int`) and floating point numbers (`number`). These can be grouped into 1-dimensional (`ivector` and `vector`) and 2-dimensional (`imatrix` and `matrix`) arrays. The 'i' in `ivector` distinguishes a vector of type `int` from a vector of type `number`. For arrays of type `number`, there are currently arrays up to dimension 7.

Some of your data must be read in from somewhere—that is, you need to start with something. These data objects are referred to as "initial objects" and are distinguished by the prefix `init`, as in `init_int` or `init_number`. All objects prefaced with `init` in the `DATA_SECTION` are read in from a data file in the order in which they are declared. The default file names for various files are derived from the name of the executable program. For example, if the executable file is named `ROOT.EXE`, then the default input data file name is `ROOT.DAT`. For this example, the executable file is named `SIMPLE.EXE`, so the default data file is `SIMPLE.DAT`. Notice that once an object has been read in, its value is available to be used to describe other data objects. In this case, the value of `nobs` can be used to define the size of the vectors `Y` and `x`. The next line

```
  init\_vector Y(1,nobs)
```

defines an initial vector object `Y` whose minimum valid index is 1 and whose maximum valid index is `nobs`. This vector object will be read in next from the data file. The contents of the file `SIMPLE.DAT` are shown below.

```
# number of observations
    10
# observed Y values
   1.4  4.7  5.1  8.3  9.0  14.5  14.0  13.4  19.2  18
# observed x values
   -1  0 1  2  3  4  5  6  7  8
```

It is possible to put comment lines in the data files. Comment lines must have the character # in the first column.

It is often useful to have data objects that are not initial. Such objects have their values calculated from the values of initial data objects. Examples of the use of non-initial data objects are given below.

1.7 The parameter section

It is the parameters of your model that provide the analysis of the data. (Perhaps more correctly, it is the values of these parameters, as picked by the fitting criterion for the model, that provide the analysis of the data.) The `PARAMETER_SECTION` is used to describe the structure of the parameters in your model. The description of the model parameters is similar to that used for the data in the `DATA_SECTION`.

All parameters are floating point numbers (or arrays of floating point numbers). The statement `init_number b` defines a floating point (actually, a double) number. The preface `init` means that this is an initial parameter. Initial parameters have two properties that distinguish them from other model parameters. First, all of the other model parameters are calculated from the initial parameters. This means that in order to calculate the values of the model parameters, it is first necessary to have values for the initial parameters. A major difference between initial data objects (which must be read in from a data file) and initial parameters is that since parameters are estimated in the model, it is possible to assign initial default values to them.

The default file name for the file that contains initial values for the initial model parameters is `ROOT.PIN`. If no file named `ROOT.PIN` is found, default values are supplied for the initial parameters. (Methods for changing the default values for initial parameters are described below.) The statement

```
vector pred_Y(1,nobs)
```

defines a vector of parameters. Since it is not prefaced with `init`, the values for this vector will not be read in from a file or given default values. It is expected that the value of the elements of this vector will be calculated in terms of other parameters.

The statement `objective_function_value f` defines a floating point (again, actually a double) number. It will hold the value of the fitting criterion. The parameters of the model are chosen so that this value is minimized.[1] Every AD Model Builder template must include a declaration of an object of type `objective_function_value` and this object must be set equal to a fitting criterion. (Don't worry. For many models, the fitting criterion is provided for you—as in the `regression` and `robust_regression` fitting criterion functions in the current and next examples.)

1.8 The procedure section

The `PROCEDURE_SECTION` contains the actual model calculations. This section contains C++ code, so C++ syntax must be obeyed. (Those familiar with C or C++ will notice that the usual methods for defining and ending a function are not necessary and, in fact, cannot be used for the routine in the main part of this section.) Statements must end with a "`;`"—exactly as with C or C++. The '`;`' is optional in the `DATA_SECTION` and the `PARAMETER_SECTION`. The code uses AUTODIF's vector operations, which enable you to avoid writing a lot of code

[1] Thus it should be set equal to minus the log-likelihood function if that criterion is used

for loops. In the statement `pred_Y=a*x+b;` the expression `a*x` forms the product of the number `a` and the components of the vector `x`, while `+b` adds the value of the number `b` to this product, so that `pred_Y` has the components $ax_i + b$. In the line

```
f=regression(Y,pred\_Y);
```

the function `regression` calculates the log-likelihood function for the regression and assigns this value to the object `f`, which is of type `objective_function_value`. This code generalizes immediately to nonlinear regression models and can be trivially modified (with the addition of one word) to perform the robust nonlinear regression. This is discussed in the second example. For the reader who wants to know, the form of the regression function is described in Appendix A.

Note that the vector of observed values goes first. The use of the `regression` function makes the purpose of the calculations clearer, and it prepares the way for modifying the routine to use AD Model Builder's robust regression function.

1.9 The preliminary calculations section

Note that `LOCAL_CALCS` and its variants in the `DATA_SECTION` and the `PROCEDURE_SECTION` has greatly reduced the need for the `PRELIMINARY_CALCS_SECTION`.

The `PRELIMINARY_CALCS_SECTION`, as its name implies, permits one to do preliminary calculations with the data before getting into the model proper. Often the input data are not in a convenient form for doing the analysis and one wants to carry out some calculations with the input data to put them in a more convenient form. Suppose that the input data for the simple regression model are in the form

```
# number of observations
    10
# observed Y values observed x values
   1.4                  -1
   4.7                   0
   5.1                   1
   8.3                   2
   9.0                   3
   14.5                  4
   14.0                  5
   13.4                  6
   19.2                  7
   18                    8
```

The problem is that the data are in pairs in the form (Y_i, x_i), so that we can't read in either the x_i or Y_i first. To read in the data in this format, we will define a matrix with `nobs` rows and two columns. The `DATA_SECTION` becomes

```
DATA_SECTION
```

```
  init_int nobs
  init_matrix Obs(1,nobs,1,2)
  vector Y(1,nobs)
  vector x(1,nobs)
```

Notice that since we do not want to read in `Y` or `x`, these objects are no longer initial objects, so their declarations are no longer prefaced with `int`. The observations will be read into the initial matrix object `Obs` so that `Y` is in the first column of `Obs`, while `x` is in the second column. If we don't want to change the rest of the code, the next problem is to get the first column of `Obs` into `Y`, and the second column of `Obs` into `x`. The following code in the `PRELIMINARY_CALCS_SECTION` will accomplish this objective. It uses the function `column`, which extracts a column from a matrix object so that it can be put into a vector object.

```
PRELIMINARY_CALCS_SECTION
 Y=column(Obs,1); // extract the first column
 x=column(Obs,2); // extract the second column
```

1.10 The use of loops and element-wise operations

This section can be skipped on first reading.

To accomplish the column-wise extraction presented above, you would have to know that AUTODIF provides the `column` operation. What if you didn't know that and don't feel like reading the manual yet? For those who are familiar with C, it is generally possible to use lower level "C-like" operations to accomplish the same objective as AUTODIF's array and matrix operations. In this case, the columns of the matrix `Obs` can also be copied to the vectors `x` and `Y` by using a standard for loop and the following element-wise operations

```
PRELIMINARY_CALCS_SECTION
  for (int i=1;i<=nobs;i++)
  {
    Y[i]=Obs[i][1];
    x[i]=Obs[i][2];
  }
```

Incidentally, the C-like operation `[]` was used for indexing members of arrays. AD Model Builder also supports the use of `()`, so that the above code could be written as

```
PRELIMINARY_CALCS_SECTION
  for (int i=1;i<=nobs;i++)
  {
    Y(i)=Obs(i,1);
    x(i)=Obs(i,2);
  }
```

which may be more readable for some users. Notice that it is also possible to define C objects, such as the object of type `int i` used as the index for the for loop, "on the fly" in the PRELIMINARY_CALCS_SECTION or the PROCEDURE_SECTION.

1.11 The default output from AD Model Builder

By default, AD Model Builder produces three or more files:

1. ROOT.PAR, which contains the parameter estimates in ASCII format,
2. ROOT.BAR, which is the parameter estimates in a binary file format, and
3. ROOT.COR, which contains the estimated standard deviations and correlations of the parameter estimates.

The template code for the simple model is in the file SIMPLE.TPL. The input data is in the file SIMPLE.DAT. The parameter estimates are in the file SIMPLE.PAR. By default, the standard deviations and the correlation matrix for the model parameters are estimated. They are in the file SIMPLE.COR:

```
 index      value      std.dev      1       2
   1   a  1.9091e+00 1.5547e-01     1
   2   b  4.0782e+00 7.0394e-01 -0.773     1
```

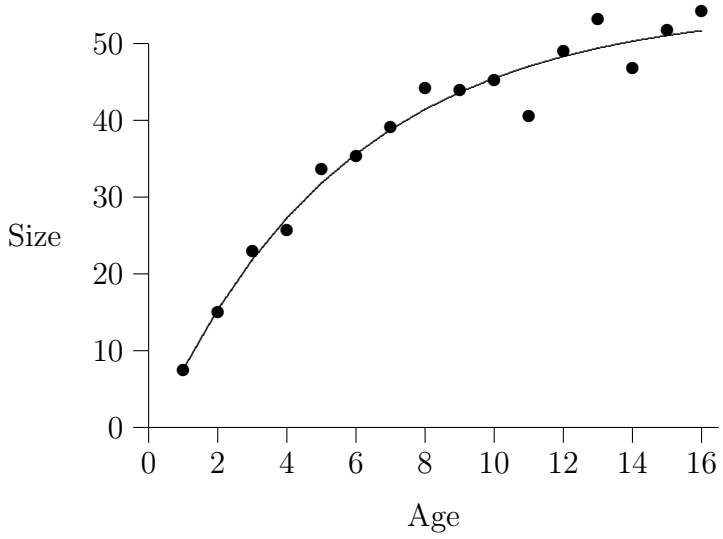
The format of the standard deviations report is to give the name of the parameter followed by its value and standard deviation. After that, the correlation matrix for the parameters is given.

1.12 Robust nonlinear regression with AD Model Builder

The code for the model template for this example is found in the file VONB.TPL. This example is intended to demonstrate the advantages of using AD Model Builder's robust regression routine over standard nonlinear least square regression procedures. Further discussion about the underlying theory can be found in the AUTODIF user's manual, but it is not necessary to understand the theory to make use of the procedure. Figure 1.1 estimates the parameters describing a growth curve from a set of data consisting of ages and size-at-age data. The form of the (von Bertalanffy) growth curve is assumed to be

$$s(a) = L_\infty \Big(1 - \exp\big(- K(a - t_0)\big) \Big) \tag{1.3}$$

The three parameters of the curve to be estimated are L_∞, K, and t_0.



index		value	std.dev	1	2	3
1	Linf	5.4861e+01	2.4704e+00	1.0000		
2	K	1.7985e-01	2.7127e-02	-0.9191	1.0000	
3	t0	1.8031e-01	2.9549e-01	-0.5856	0.7821	1.0000

Figure 1.1: Results for nonlinear regression with good data set.

Let O_i and a_i be the observed size and age of the i^{th} animal. The predicted size $s(a_i)$ is given by equation (1.3). The least-squares estimates for the parameters are found by minimizing

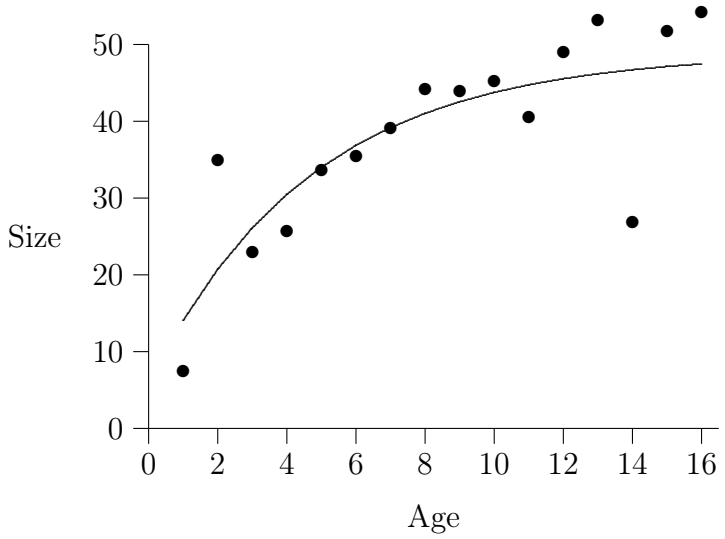
$$\min_{L_\infty,K,t_0} \sum_i \big(O_i - s(a_i)\big)^2$$

```
DATA_SECTION
  init_int nobs;
  init_matrix data(1,nobs,1,2)
  vector age(1,nobs);
  vector size(1,nobs);
PARAMETER_SECTION
  init_number Linf;
  init_number K;
  init_number t0;
  vector pred_size(1,nobs)
  objective_function_value f;
PRELIMINARY_CALCS_SECTION
  // get the data out of the columns of the data matrix
  age=column(data,1);
  size=column(data,2);
  Linf=1.1*max(size); // set Linf to 1.1 times the longest observed length
PROCEDURE_SECTION
  pred_size=Linf*(1.-exp(-K*(age-t0)));
  f=regression(size,pred_size);
```

Notice the use of the `regression` function, which calculates the log-likelihood function of the nonlinear least-squares regression. This part of the code is formally identical to the code for the linear regression problem in the simple example, even though we are now doing nonlinear regression. A graph of the least-square estimated growth curve and the observed data is given in Figure 1.1. The parameter estimates and their estimated standard deviations produced by AD Model Builder are also given. For example, the estimate for L_∞ is 54.86, with a standard deviation of 2.47. Since a 95% confidence limit is about $\pm$ two standard deviations, the usual 95% confidence limit of L_∞ for this analysis would be 54.86 ± 4.94.

A disadvantage of least-squares regression is the sensitivity of the estimates to a few "bad" data points or outliers. Figure 1.2 shows the least-squares estimates when the observed size for age 2 and age 14 have been moved off the curve. There has been a rather large change in some of the parameter estimates. For example, the estimate for L_∞ has changed from 54.86 to 48.91, and the estimated standard deviation for this parameter has increased to 5.99. This is a common effect of outliers on least-squares estimates. They greatly increase the size of the estimates of the standard deviations. As a result, the confidence limits for the parameters are increased. In this case, the 95% confidence limits for L_∞ have been increased from 54.86 ± 4.94 to 48.91 ± 11.98.

Of course, for this simple example, it could be argued that a visual examination of the residuals would identify the outliers so that they could be removed. This is true, but in larger nonlinear models, it is often not possible, or convenient, to identify and remove all the outliers in this fashion. Also, the process of removing "inconvenient" observations from data can be uncomfortably close to "cooking" the data in order to obtain the desired result from the analysis. An alternative approach, which avoids these difficulties, is to employ AD Model Builder's robust regression procedure, which removes the undue influence of outlying points without the need to expressly remove them from the data.




```
Nonlinear regression with bad data set
index        value     std.dev      1      2      3
   1   Linf  4.8905e+01 5.9938e+00 1.0000
   2   K     2.1246e-01 1.2076e-01 -0.8923 1.0000
   3   t0   -5.9153e-01 1.4006e+00 -0.6548 0.8707 1.0000
```

Figure 1.2: Nonlinear regression with bad data set.

1.13 Modifying the model to use robust nonlinear regression

To invoke the robust regression procedure, it is necessary to make three changes to the existing code. The template for the robust regression version of the model can be found in the file `VONBR.TPL`.

```
DATA_SECTION
  init_int nobs;
```

```
  init_matrix data(1,nobs,1,2)
  vector age(1,nobs)
  vector size(1,nobs)
PARAMETER_SECTION
  init_number Linf
  init_number K
  init_number t0
  vector pred_size(1,nobs)
  objective_function_value f
  init_bounded_number a(0.0,0.7,2)
PRELIMINARY_CALCS_SECTION
  // get the data out of the columns of the data matrix
  age=column(data,1);
  size=column(data,2);
  Linf=1.1*max(size); // set Linf to 1.1 times the longest observed length
  a=0.7;
PROCEDURE_SECTION
  pred_size=Linf*(1.-exp(-K*(age-t0)));
  f=robust_regression(size,pred_size,a);
```

The main modification to the model involves the addition of the parameter `a`, which is used to estimate the amount of contamination by outliers. This parameter is declared in the `PARAMETER_SECTION`:

```
  init_bounded_number a(0.0,0.7,2)
```

This introduces two concepts: 1) putting bounds on the values that initial parameters can take on and 2) carrying out the minimization in a number of stages. The value of `a` should be restricted to lie between 0.0 and 0.7. (See the discussion on robust regression in the AUTODIF user's manual if you want to know where the 0.0 and 0.7 come from.) This is accomplished by declaring `a` to be of type `init_bounded_number`. In general, it is not possible to estimate the parameter `a` determining the amount of contamination by outliers until the other parameters of the model have been "almost" estimated—that is, until we have done a preliminary fit of the model. This is a common situation in nonlinear modeling and is discussed further in some later examples. So, we want to carry out the minimization in two phases.

During the first phase, `a` should be held constant. In general, for any initial parameter, the last number in its declaration, if present, determines the number of the phase in which that parameter becomes active. If no number is given, the parameter becomes active in phase 1. *Note:* For an `init_bounded_number`, the upper and lower bounds must be given, so the declaration

```
  init_bounded_number a(0.0,0.7)
```

would use the default phase 1. The `2` in the declaration for `a` causes `a` to be constant until the second phase of the minimization.

The second change to the model involves the default initial value `a`. The default value for a bounded number is the average of the upper and lower bounds. For `a`, this would be 0.35, which is too small. We want to use the upper bound of 0.7. This is done by adding the line

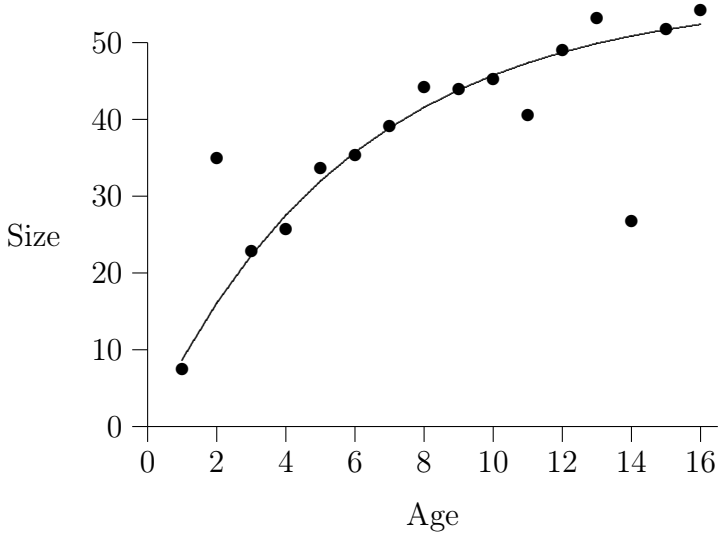
```
a=0.7;
```

in the `PRELIMINARY_CALCS_SECTION`. Finally, we modify the statement in the `PROCEDURE_SECTION` that includes the `regression` function to be

```
f=robust_regression(size,pred_size,a);
```

to invoke the robust regression function.

That's all there is to it! These three changes will convert any AD Model builder template from a nonlinear regression model to a robust nonlinear regression model.

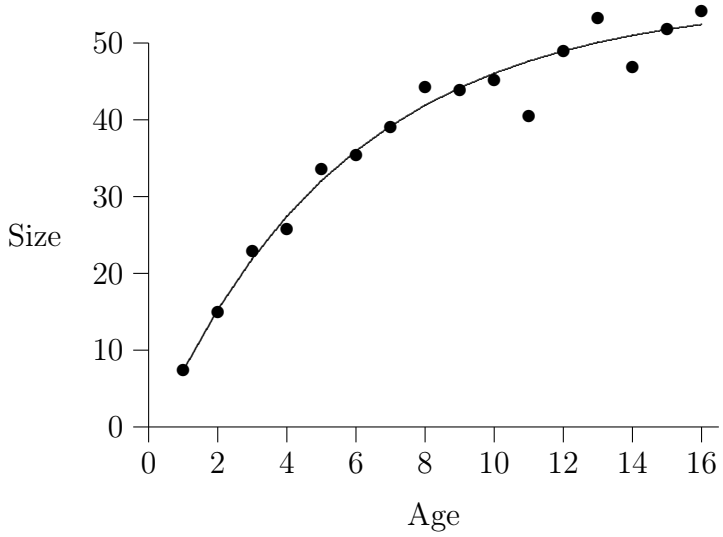


index		value	std.dev	1	2	3	4
1	Linf	5.6184e+01	3.6796e+00	1.0000			
2	K	1.6818e-01	3.4527e-02	-0.9173	1.0000		
3	t0	6.5129e-04	4.5620e-01	-0.5483	0.7724	1.0000	
4	a	3.6144e-01	1.0721e-01	-0.1946	0.0367	-0.2095	1.0000

Figure 1.3: Robust Nonlinear regression with bad data set.

The results for the robust regression fit to the bad data set are shown in Figure 1.3. The estimate for L_∞ is 56.18, with a standard deviation of 3.68, to give a 95% confidence interval of about 56.18 ± 7.36. Both the parameter estimates and the confidence limits are much less affected by the outliers for the robust regression estimates than they are for the least-squares estimates. The parameter `a` is estimated to be equal to 0.36, which indicates that the robust procedure has detected some moderately large outliers.

The results for the robust regression fit to the good data set are shown in Figure 1.4. The estimates are almost identical to the least-square estimates for the same data. This is a property of the robust estimates. They do almost as well as the least-square estimates when the assumption of normally distributed errors in the statistical model is satisfied exactly. They do much better than least-square estimates in the presence of moderate or large outliers. You can lose only a little and you stand to gain a lot by using these estimators.



index		value	std.dev	1	2	3	4
1	Linf	5.5707e+01	1.9178e+00	1.0000			
2	K	1.7896e-01	1.9697e-02	-0.9148	1.0000		
3	t0	2.1490e-01	2.0931e-01	-0.5604	0.7680	1.0000	
4	a	7.0000e-01	3.2246e-05	-0.0001	0.0000	-0.0000	1.0000

Figure 1.4: Robust Nonlinear regression with good data set.

1.14 Chemical engineering: a chemical kinetics problem

This example may strike you as being fairly complicated. If so, you should compare it with the original solution using the so-called sensitivity equations. The reference is [1], Chapter 8. We consider the chemical kinetics problem introduced on page 233. This is a model defined by a first order system of two ordinary differential equations.

$$ds_1/dt = -\theta_1 \exp\big(-\theta_2/T\big)\big(s_1 - e^{-1000/T} s_2^2\big)/\big(1 + \theta_3 \exp(-\theta_4/T) s_1\big)^2$$
$$ds_2/dt = 2\theta_1 \exp\big(-\theta_2/T\big)\big(s_1 - e^{-1000/T} s_2^2\big)/\big(1 + \theta_3 \exp(-\theta_4/T) s_1\big)^2$$

(1.4)

The differential equations describe the evolution over time of the concentrations of the two reactants, s_1 and s_2. There are 10 initial parameters in the model: $\theta_1, \ldots, \theta_{10}$. T is the temperature at which the reaction takes place. To integrate the system of differential equations, we require the initial concentrations of the reactants: $s_1(0)$ and $s_2(0)$ at time zero.

The reaction was carried out three times at temperatures of 200, 400, and 600 degrees. For the first run, there were initially equal concentrations of the two reactants. The second run initially consisted of only the first reactant, and the third run initially consisted of only the second reactant. The initial concentrations of the reactants are known only approximately. See Table 1.1 for what they are. The unknown initial concentrations are treated as

Run 1	$s_1(0) = \theta_5 = 1 \pm 0.05$	$s_2(0) = \theta_6 = 1 \pm 0.05$
Run 2	$s_1(0) = \theta_7 = 1 \pm 0.05$	$s_2(0) = 0$
Run 3	$s_1(0) = 0$	$s_2(0) = \theta_8 = 1 \pm 0.05$

Table 1.1

parameters to be estimated with Bayesian prior distributions on them, reflecting the level of certainty of their true values that we have. The concentrations of the reactants were not measured directly. Rather, the mixture was analyzed by a "densitometer," whose response to the concentrations of the reactants is

$$y = 1 + \theta_9 s_1 + \theta_{10} s_2$$

where $\theta_9 = 1 \pm 0.05$ and $\theta_{10} = 2 \pm 0.05$. The differences between the predicted and observed responses of the densitometer are assumed to be normally distributed, so least squares is used to fit the model. Bard employs an "explicit" method for integrating these differential equations, that is, the equations are approximated by a finite difference scheme, such as

$$\begin{aligned} s_1(t_{n+1}) &= s_1(t_n) - h\theta_1 \frac{\exp\big(-\theta_2/T\big)\big(s_1(t_n) - e^{-1000/T} s_2(t_n)^2\big)}{\big(1 + \theta_3 \exp(-\theta_4/T) s_1(t_n)\big)^2} \\ s_2(t_{n+1}) &= s_2(t_n) + 2h\theta_1 \frac{\exp\big(-\theta_2/T\big)\big(s_1(t_n) - e^{-1000/T} s_2(t_n)^2\big)}{\big(1 + \theta_3 \exp(-\theta_4/T) s_1(t_n)\big)^2} \end{aligned} \tag{1.5}$$

over the time period t_n to t_{n+1} of length h. Equations (1.5) are called "explicit," because the values of s_1 and s_2 at time t_{n+1} are given explicitly in terms of the values of s_1 and s_2 at time t_n.

The advantage of using an explicit scheme for integrating the model differential equations is that the derivatives of the model functions with respect to the model parameters also satisfy differential equations. They are called "sensitivity equations" (see [1], pages 227–229). It is possible to integrate these equations, as well as the model equations, to get values for the

derivatives. However, this involves generating a lot of extra code, as well as carrying out a lot of extra calculations. Since with AD Model Builder it is not necessary to produce any code for derivative calculations, it is possible to employ alternate schemes for integrating the differential equations.

Let $A = \theta_1 \exp(-\theta_2/T)$, $B = \exp(-1000/T)$, and $C = (1 + \theta_3 \exp(-\theta_4/T)s_1)^2$. In terms of A and C, we can replace the explicit finite difference scheme by the semi-implicit scheme

$$\begin{aligned} s_1(t_{n+1}) &= s_1(t_n) - hA\big(s_1(t_{n+1}) - Bs_2^2(t_{n+1})\big)/C \\ s_2(t_{n+1}) &= s_2(t_n) + 2hA\big(s_1(t_{n+1}) - Bs_2(t_n)s_2(t_{n+1})\big)/C \end{aligned} \tag{1.6}$$

Now let $D = hA/C$ and solve equations (3) for $s_1(t_{n+1})$ and $s_2(t_{n+1})$ to obtain

$$\begin{aligned} s_1(t_{n+1}) &= \big(s_1(t_n) + DBs_2(t_n)\big)/(1 + D) \\ s_2(t_{n+1}) &= \big(s_2(t_n) + 2Ds_1(t_n)\big)/\big(1 + (2DBs_2(t_n))\big) \end{aligned} \tag{1.7}$$

Implicit and semi-implicit schemes tend to be more stable than explicit schemes over large time steps and large values of some of the model parameters. This stability is especially important when fitting nonlinear models, because the algorithms for function minimization will pick very large, or "bad," values of the parameters from time to time, and the minimization procedure will generally perform better when a more stable scheme is employed.

```
DATA_SECTION
  init_matrix Data(1,10,1,3)
  init_vector T(1,3) // the initial temperatures for the three runs
  init_vector stepsize(1,3) // the stepsize to use for numerical integration
  matrix data(1,3,1,10)
  matrix sample_times(1,3,1,10) // times at which reaction was sampled
  vector x0(1,3)         // the beginning time for each of the three
                         // runs
  vector x1(1,3)         // the ending time for each of the three runs
  // for each of the three runs

PARAMETER_SECTION
  init_vector theta(1,10) // the model parameters
  matrix init_conc(1,3,1,2) // the initial concentrations of the two
                          // reactants over three time periods
  vector instrument(1,2) // determines the response of the densitometer
  matrix y_samples(1,10,1,2)// the predicted concentrations of the two
                          // reactants at the ten sampling periods
                          // obtained by integrating the differential
                          // equations
  vector diff(1,10)       // the difference between the observed and
                          // readings of the densitometer
```

```
  objective_function_value f // the log_likelihood function
  number bayes_part      // the Bayesian contribution
  number y2
  number x_n
  vector y_n(1,2)
  vector y_n1(1,2)
  number A // A B C D hold some common subexpressions
  number B
  number C
  number D
PRELIMINARY_CALCS_SECTION
  data=trans(Data); // it is more convenient to work with the transformed
                    // matrix
PROCEDURE_SECTION

    // set up the begining and ending times for the three runs
    x0(1)=0;
    x1(1)=90;
    x0(2)=0;
    x1(2)=18;
    x0(3)=0;
    x1(3)=4.5;
    // set up the sample times for each of the three runs
    sample_times(1).fill_seqadd(0,10); // fill with 0,10,20,...,90
    sample_times(2).fill_seqadd(0,2); // fill with 0,2,4,...,18
    sample_times(3).fill_seqadd(0,0.5); // fill with 0,0.5,1.0,...,4.5

    // set up the initial concentrations of the two reactants for
    // each of the three runs
    init_conc(1,1)=theta(5);
    init_conc(1,2)=theta(6);
    init_conc(2,1)=theta(7);
    init_conc(2,2)=0.0;   // the initial concentrations is known to be 0
    init_conc(3,1)=0.0;   // the initial concentrations is known to be 0
    init_conc(3,2)=theta(8);

    // coefficients which determine the response of the densitometer
    instrument(1)=theta(9);
    instrument(2)=theta(10);
    f=0.0;
    for (int run=1;run<=3;run++)
    {
```

```
   // integrate the differential equations to get the predicted
   // values for the y_samples
  int nstep=(x1(run)-x0(run))/stepsize(run);
  nstep++;
  double h=(x1(run)-x0(run))/nstep; // h is the stepsize for integration

  int is=1;
  // get the initial conditions for this run
  x_n=x0(run);
  y_n=init_conc(run);
  for (int i=1;i<=nstep+1;i++)
  {
    // gather common subexpressions
    y2=y_n(2)*y_n(2);
    A=theta(1)*exp(-theta(2)/T(run));
    B=exp(-1000/T(run));
    C=(1+theta(3)*exp(-theta(4)/T(run))*y_n(1));
    C=C*C;
    D=h*A/C;
    // get the y vector for the next time step
    y_n1(1)=(y_n(1)+D*B*y2)/(1.+D);
    y_n1(2)=(y_n(2)+2.*D*y_n(1))/(1.+(2*D*B*y_n(2)));

    // if an observation occurred during this time period save
    // the predicted value
    if (is <=10)
    {
      if (x_n<=sample_times(run,is) && x_n+h >= sample_times(run,is))
      {
        y_samples(is++)=y_n;
      }
    }
    x_n+=h; // increment the time step
    y_n=y_n1; // update the y vector for the next step

  }
  diff=(1.0+y_samples*instrument)-data(run); //differences between the
            // predicted and observed values of the densitometer
  f+=diff*diff; // sum of squared differences
}
// take the log of f and multiply by nobs/2 to get log-likelihood
f=15.*log(f); // This is (number of obs)/2. It is wrong in Bard (pg 236).
```

```
// Add the Bayesian stuff
bayes_part=0.0;
for  (int i=5;i<=9;i++)
{
  bayes_part+=(theta(i)-1)*(theta(i)-1);
}
bayes_part+=(theta(10)-2)*(theta(10)-2);
f+=1./(2.*.05*.05)*bayes_part;
```

AD Model Builder produces a report containing values, standard deviations, and correlation matrix of the parameter estimates. As discussed below, any parameter or group of parameters can easily be included in this report. For models with a large number of parameters, this report can be a bit unwieldly, so options are provided to exclude parameters from the report, if desired.

index		value	std.dev	1	2	3	4	5	6	7	8	9	10
1	theta	1.37e+00	2.09e-01	1									
2	theta	1.12e+03	7.70e+01	0.95	1								
3	theta	1.80e+00	7.95e-01	0.9	0.98	1							
4	theta	3.58e+02	1.94e+02	0.91	0.98	0.99	1						
5	theta	1.00e+00	4.49e-02	0.20	0.28	0.12	0.17	1					
6	theta	9.94e-01	2.99e-02	-0.42	-0.35	-0.25	-0.22	-0.58	1				
7	theta	9.86e-01	2.59e-02	0.01	0.22	0.22	0.28	0.26	0.42	1			
8	theta	1.02e+00	1.69e-02	-0.38	-0.34	-0.36	-0.30	0.09	0.63	0.34	1		
9	theta	1.00e+00	2.59e-02	-0.02	-0.23	-0.23	-0.30	-0.28	-0.43	-0.98	-0.37	1	
10	theta	1.97e+00	3.23e-02	0.44	0.37	0.40	0.32	-0.09	-0.65	-0.37	-0.93	0.40	1

1.15 Financial Modelling: a generalized autoregressive conditional heteroskedasticity or GARCH model

Time series models are often used in financial modeling. For these models, the parameters are often extremely badly determined. With the stable numerical environment produced by AD Model Builder, it is a simple matter to fit such models.

Consider a time series of returns r_t, where $t = 0, \ldots, T$, available from some type of financial instrument. The model assumptions are

$$r_t = \mu + \epsilon_t \quad h_t = a_0 + a_1 \epsilon_{t-1}^2 + a_2 h_{t-1} \qquad \text{for } \; 1 \le t \le T, \;\; a_0 \ge 0, \;\; a_1 \ge 0, \;\; a_2 \ge 0$$

where the ϵ_t are independent normally distributed random variables with mean 0 and variance h_t. We assume $\epsilon_0 = 0$ and $h_0 = \sum_{i=0}^{T} (r_i - \bar{r})^2/(T+1)$. There are four initial parameters to be estimated for this model: μ, a_0, a_1, and a_2. The log-likelihood function for the vector r_t is equal to a constant plus

$$-.5 \sum_{t=1}^{T} \left(\log(h_t) + (r_t - \mu)^2/h_t \right)$$

```
DATA_SECTION
  init_int T
  init_vector r(0,T)
  vector sub_r(1,T)
  number h0
INITIALIZATION_SECTION
  a0 .1
  a1 .1
  a2 .1
PARAMETER_SECTION
  init_bounded_number a0(0.0,1.0)
  init_bounded_number a1(0.0,1.0,2)
  init_bounded_number a2(0.0,1.0,3)
  init_number Mean
  vector eps2(1,T)
  vector h(1,T)
  objective_function_value log_likelihood
PRELIMINARY_CALCS_SECTION
  h0=square(std_dev(r)); // square forms the element-wise square
  sub_r=r(1,T);  // form a subvector so we can use vector operations
  Mean=mean(r);  // calculate the mean of the vector r
PROCEDURE_SECTION
  eps2=square(sub_r-Mean);
  h(1)=a0+a2*h0;
  for (int t=2;t<=T;t++)
  {
    h(t)=a0+a1*eps2(t-1)+a2*h(t-1);
  }
  // calculate minus the log-likelihood function
  log_likelihood=.5*sum(log(h)+elem_div(eps2,h)); // elem_div performs
                              // element-wise division of vectors
RUNTIME_SECTION
  convergence_criteria .1, .1, .001
  maximum_function_evaluations 20, 20, 1000
```

We have used vector operations such as `elem_div` and `sum` to simplify the code. Of course, the code could also have employed loops and element-wise operations. The parameter values and standard deviation report for this model appears below.

```
 index        value     std.dev      1      2      3      4
   1   a0    1.6034e-04 2.3652e-05 1.0000
   2   a1    9.3980e-02 2.0287e-02 0.1415 1.0000
   3   a2    3.7263e-01 8.2333e-02 -0.9640 -0.3309 1.0000
   4   Mean -1.7807e-04 3.0308e-04 0.0216 -0.1626 0.0144 1.0000
```

This example employs bounded initial parameters. Often it is necessary to put bounds on parameters in nonlinear modeling, to ensure that the minimization is stable. In this example, a0 is constrained to lie between 0.0 and 1.0:

```
init_bounded_number a0(0.0,1.0)
init_bounded_number a1(0.0,1.0,2)
init_bounded_number a2(0.0,1.0,3)
```

1.16 Carrying out the minimization in a number of phases

For linear models, one can simply estimate all the model parameters simultaneously. For nonlinear models, often this simple approach does not work very well. It may be necessary to keep some of the parameters fixed during the initial part of the minimization process, and carry out the minimization over a subset of the parameters. The other parameters are included into the minimization process, in a number of phases until all of the parameters have been included. AD Model Builder provides support for this multi-phase approach. In the declaration of any initial parameter, the last number, if present, determines the phase of the minimization during which this parameter is included (becomes active). If no number is present, the initial parameter becomes active in phase 1. In this case, a0 has no phase number and so becomes active in phase 1. a1 becomes active in phase 2, and a2 becomes active in phase 3. In this example, phase 3 is the last phase of the optimization.

It is often convenient to modify aspects of the code depending on what phase of the minimization procedure is the current phase, or on whether a particular initial parameter is active. The function

```
current_phase()
```

returns an integer (an object of type int) that is the value of the current phase. The function

```
last_phase()
```

returns the value "true" ($\neq 0$) if the current phase is the last phase and false ($= 0$) otherwise. If xxx is the name of any initial parameter the function

```
active(xxx)
```

returns the value "true" if xxx is active during the current phase and false otherwise.

After the minimization of the objective function has been completed, AD Model Builder calculates the estimated covariance matrix for the initial parameters, as well as any other desired parameters that have been declared to be of sd_report type. Often, these additional parameters may involve considerable additional computational overhead. If the values of these parameters are not used in calculations proper, it is possible to only calculate them during the standard deviations report phase.

```
sd_phase()
```

The `sd_phase` function returns the value "true" if we are in the standard deviations report phase and "false" otherwise. It can be used in a conditional statement to determine whether to perform calculations associated with some `sd_report` object.

When estimating the parameters of a model by a multi-phase minimization procedure, the default behavior of AD Model Builder is to carry out the default number of function evaluations until convergence is achieved in each stage. If we are only interested in the parameter estimates obtained after the last stage of the minimization, it is often not necessary to carry out the full minimization in each stage. Sometimes, considerable time can be saved by relaxing the convergence criterion in the initial stages of the optimization.

The `RUNTIME_SECTION` allows the user to modify the default behavior of the function minimizer during the phases of the estimation process:

```
RUNTIME_SECTION
  convergence_criteria .1, .1, .001
  maximum_function_evaluations 20, 20, 1000
```

The `convergence_criteria` affects the criterion used by the function minimizer to decide when the optimization process has occurred. The function minimizer compares the maximum value of the vector of derivatives of the objective function, with respect to the independent variables, to the numbers after the `convergence_criteria` keyword. The first number is used in the first phase of the optimization, the second number in the second phase, and so on. If there are more phases to the optimization than there are numbers, the last number is used for the rest of the phases of the optimization. The numbers must be separated by commas. The spaces are optional. The `maximum_function_evaluations` keyword controls the maximum number of evaluations of the objective function that will be performed by the function minimizer in each stage of the minimization procedure.

1.17 Natural resource management: the Schaefer-Pella-Tomlinson Model

It is typical of many models in natural resource management that the model tends to be rather unstable numerically. In addition, some of the model parameters are often poorly determined. Notwithstanding these difficulties, it is often necessary to make decisions about resource management based on the analysis provided by these models. This example provides a good opportunity for presenting some more advanced features of AD Model Builder that are designed to overcome these difficulties.

The Schaefer-Pella-Tomlinson model is employed in fisheries management. The model assumes that the total biomass of an exploited fish stock satisfies an ordinary differential equation of the form

$$\frac{dB}{dt} = rB\left(1 - \left(\frac{B}{k}\right)^{m-1}\right) - FB \qquad \text{where} \quad m > 1 \tag{1.8}$$

([7], page 303), where B is the biomass, F is the instantaneous fishing mortality rate, r is a parameter often referred to an the "intrinsic rate of increase," k is the unfished equilibrium stock size,

$$C = FB \tag{1.9}$$

is the catch rate, and m is a parameter that determines where the maximum productivity of the stock occurs. If the value of m is fixed at 2, the model is referred to as the "Schaefer model." The explicit form of the difference equation corresponding to this differential equation is

$$B_{t+\delta} = B_t + rB_t\delta - rB_t\left(\frac{B_t}{k}\right)^{m-1}\delta - F_tB_t\delta \tag{1.10}$$

To get a semi-implicit form of this difference equation that has better numerical stability than the explicit version, we replace some of the terms B_t on the right hand side of 1.10 by $B_{t+\delta}$, to get

$$B_{t+\delta} = B_t + rB_t\delta - rB_{t+\delta}\left(\frac{B_t}{k}\right)^{m-1}\delta - F_tB_{t+\delta}\delta \tag{1.11}$$

We solve for $B_{t+\delta}$ to give

$$B_{t+\delta} = \frac{B_t(1+r\delta)}{1+\left(r(B_t/k)^{m-1}+F_t\right)\delta} \tag{1.12}$$

The catch $C_{t+\delta}$ over the period $(t, t+\delta)$ is given by

$$C_{t+\delta} = F_tB_{t+\delta}\delta \tag{1.13}$$

1.18 Bayesian considerations in the Pella-Tomlinson Model

The parameter k is referred to as the "carrying capacity" or the "unfished equilibrium biomass level," because it is the value that the biomass of the population will eventually assume if there is no fishing. For a given value of k, the parameter m determines the level of maximum productivity—that is, the level of biomass $B_{\rm MAX}$ for which the removals from fishing can be the greatest:

$$B_{\rm MAX} = \frac{k}{\sqrt[m-1]{m}}$$

For $m = 2$, maximum productivity is obtained by that level of fishing pressure that reduces the stock to 50% of the carrying capacity. For the data available in many real fisheries problems, the parameter m is very poorly determined. It is common practice, therefore, to simply assume that $m = 2$. Similarly, it is commonly assumed that the carrying capacity k does not change over time, even though changes such as habitat degradation may well lead to changes in k.

We want to construct a statistical model where the carrying capacity can be varying slowly over time if there appears to be any information in the fisheries data supporting this

hypothesis. What is meant by "slowly"? The answer to this question will depend on the particular situation. For our purposes, "slowly" means "slowly enough" so that the model has some chance of supplying a useful analysis of the situation at hand. We refer to this as "the assumption of manageability." The point is that since we are going to use this model anyways to try and manage a resource, we may as well assume that the model's assumptions are satisfied—at least well enough that we have some hope of success. This may seem extremely arbitrary, and it is. However, it is not as arbitrary as assuming that the carrying capacity is constant.

We assume that $k_{i+1} = k_i \exp(\kappa_i)$, where the κ_i are independent normally distributed random variables with mean 0, and that $\log(m-1)$ is normally distributed with mean 0. The parameters $\log(k)$ are assumed to have the structure of a random walk, which is the simplest type of time series. This Bayesian approach is a very simple method for including a time series structure into the parameters of a nonlinear model.

We don't know the true catches C_i in each year. What we have are estimates C_i^{obs} of the catch. We assume that the quantities $\log(C_i^{obs}/C_i)$ are normally distributed with mean 0.

Finally, we must deal with the fishing mortality F. Estimates of F are not obtained directly. Instead, what is observed is an index of fishing mortality—in this case, fishing effort. We assume that for each year, we have an estimate E_i of fishing effort and that the fishing mortality rate F_i in year i satisfies the relationship $F_i = qE_i \exp(\eta_i)$, where q is a parameter referred to as the "catchability" and the η_i are normally distributed random variables with mean 0.

We assume that the variance of the η_i is 10 times the variance in the observed catch errors, and that the variance of the κ_i is 0.1 times the variance in the observed catch errors. We assume that the variance in $\log(m-1)$ is 0.25. Then, given the data, the Bayesian posterior distribution for the model parameters is proportional to

$$-(3n-1)/2 \log\left(\sum_{i=1}^{n}\big(\log(C_i^{obs}) - \log(C_i)\big)^2 + .1\sum_{i=1}^{n}\eta_i^2 + 10\sum_{i=2}^{n}\kappa_i^2\right) - 2.\log(m-1)^2 \tag{1.14}$$

The number of initial parameters in the model (that is, the number of independent variables in the function to be minimized) is $2n+4$. For the halibut data, there are 56 years of data, which gives 116 parameters. As estimates of the model parameters, we use the mode of the posterior distribution, which can by found by minimizing -1 times expression (1.14). The covariance matrix of the model parameters are estimated by computing the inverse of the Hessian of expression (1.14) at the minimum. The template for the model follows. To improve the readability, the entire template has been included. The various sections are discussed below.

```
DATA_SECTION
  init_int nobs;
  init_matrix data(1,nobs,1,3)
  vector obs_catch(1,nobs);
```

```
  vector cpue(1,nobs);
  vector effort(1,nobs);
  number avg_effort
INITIALIZATION_SECTION
  m 2.
  beta 1.
  r 1.
PARAMETER_SECTION
  init_bounded_number q(0.,1.)
  init_bounded_number beta(0.,5.)
  init_bounded_number r(0.,5,2)
  init_number log_binit(2)
  init_bounded_dev_vector effort_devs(1,nobs,-5.,5.,3)
  init_bounded_number m(1,10.,4)
  init_bounded_vector k_devs(2,nobs,-5.,5.,4)
  number binit
  vector pred_catch(1,nobs)
  vector biomass(1,nobs)
  vector f(1,nobs)
  vector k(1,nobs)
  vector k_trend(1,nobs)
  sdreport_number k_1
  sdreport_number k_last
  sdreport_number k_change
  sdreport_number k_ratio
  sdreport_number B_projected
  number tmp_mort;
  number bio_tmp;
  number c_tmp;
  objective_function_value ff;
PRELIMINARY_CALCS_SECTION
  // get the data out of the data matrix into
  obs_catch=column(data,2);
  cpue=column(data,3);
  // divide the catch by the cpue to get the effort
  effort=elem_div(obs_catch,cpue);
  // normalize the effort and save the average
  double avg_effort=mean(effort);
  effort/=avg_effort;
  cout << " beta" << beta << endl;
PROCEDURE_SECTION
  // calculate the fishing mortality
```

```
  calculate_fishing_mortality();
  // calculate the biomass and predicted catch
  calculate_biomass_and_predicted_catch();
  // calculate the objective function
  calculate_the_objective_function();

FUNCTION calculate_fishing_mortality
  // calculate the fishing mortality
  f=q*effort;
  if (active(effort_devs)) f=elem_prod(f,exp(effort_devs));

FUNCTION calculate_biomass_and_predicted_catch
  // calculate the biomass and predicted catch
  if (!active(log_binit))
  {
    log_binit=log(obs_catch(1)/(q*effort(1)));
  }
  binit=exp(log_binit);
  biomass[1]=binit;
  if (active(k_devs))
  {
    k(1)=binit/beta;
    for (int i=2;i<=nobs;i++)
    {
      k(i)=k(i-1)*exp(k_devs(i));
    }
  }
  else
  {
    // set the whole vector equal to the constant k value
    k=binit/beta;
  }
  // only calculate these for the standard deviation report
  if (sd_phase)
  {
    k_1=k(1);
    k_last=k(nobs);
    k_ratio=k(nobs)/k(1);
    k_change=k(nobs)-k(1);
  }
  // two time steps per year desired
  int nsteps=2;
```

```
  double delta=1./nsteps;
  // Integrate the logistic dynamics over n time steps per year
  for (int i=1; i<=nobs; i++)
  {
    bio_tmp=1.e-20+biomass[i];
    c_tmp=0.;
    for (int j=1; j<=nsteps; j++)
    {
      //This is the new biomass after time step delta
      bio_tmp=bio_tmp*(1.+r*delta)/
        (1.+ (r*pow(bio_tmp/k(i),m-1.)+f(i))*delta );
      // This is the catch over time step delta
      c_tmp+=f(i)*delta*bio_tmp;
    }
    pred_catch[i]=c_tmp;     // This is the catch for this year
    if (i<nobs)
    {
      biomass[i+1]=bio_tmp;// This is the biomass at the beginning of the next
    }                     // year
    else
    {
      B_projected=bio_tmp; // get the projected biomass for std dev report
    }
  }

FUNCTION calculate_the_objective_function
  if (!active(effort_devs))
  {
    ff=nobs/2.*log(norm2(log(obs_catch)-log(1.e-10+pred_catch)));
  }
  else if(!active(k_devs))
  {
    ff= .5*(size_count(obs_catch)+size_count(effort_devs))*
      log(norm2(log(obs_catch)-log(1.e-10+pred_catch))
      +0.1*norm2(effort_devs));
  }
  else
  {
    ff= .5*( size_count(obs_catch)+size_count(effort_devs)
      +size_count(k_devs) )*
      log(norm2(log(obs_catch)-log(pred_catch))
      + 0.1*norm2(effort_devs)+10.*norm2(k_devs));
```

```
  }
  // Bayesian contribution for Pella Tomlinson m
  ff+=2.*square(log(m-1.));
  if (current_phase()<3)
  {
    ff+=1000.*square(log(mean(f)/.4));
  }
```

The data are contained in three columns, with the catch and catch per unit effort data contained in the second and third columns. The matrix `data` is defined in order to read the data. The second and third columns of `data`, which is what we are interested in, will then be put into the vectors `obs_catch` and `cpue`. (Later, we get the fishing effort by dividing the `obs_catch` by the `cpue`.)

```
DATA_SECTION
  init_int nobs
  init_matrix data(1,nobs,1,3)
  vector obs_catch(1,nobs)
  vector cpue(1,nobs)
  vector effort(1,nobs)
  number avg_effort
```

The `INITIALIZATION_SECTION` is used to define default values for some model parameters if the standard default provided by AD Model Builder is not acceptable. If the model finds the parameter file (whose default name is `admodel.par`), it will read in the initial values for the parameters from there. Otherwise, the default values will be used—unless the parameters appear in the `INITIALIZATION_SECTION`, in which case, those values will be used.

```
INITIALIZATION_SECTION
  m 2.
  beta 1.
  r 1.
```

The `PARAMETER_SECTION` for this model introduces several new features of AD Model Builder. The statement

```
  init_bounded_number r(0.,5.,2)
```

declares an initial parameter whose value will be constrained to lie between 0.0 and 5.0. It is often necessary to put bounds on the initial parameters in nonlinear models to get stable model performance. This is accomplished in AD Model Builder simply by declaring the initial parameter to be bounded and providing the desired bounds. The default initial value for a bounded object is the average of the lower and upper bounds.

The third number '`2`' in the declaration determines that this initial parameter will not be made active until the second phase of the minimization. This introduces the concept of "phases" in the minimization process.

As soon as nonlinear statistical models become a bit complicated, one often finds that simply attempting to estimate all the parameters simultaneously does not work very well. In short, "You can't get there from here." A better strategy is to keep some of the parameters fixed and to first minimize the function with respect to the other parameters. More parameters are added in a stepwise relaxation process. In AD Model Builder, each step of this relaxation process is termed a "phase." The parameter `r` is not allowed to vary until the second phase. Initial parameters that are allowed to vary will be termed "active." In the first phase, the active parameter are `beta` and `q`. The default phase for an initial parameter is phase 1 if no phase number is included in its declaration. The phase number for an initial parameter is the last number in the declaration for that parameter. The general order for the arguments in the definition of any initial parameter is the size data for a vector or matrix object (if needed), the bounds for a bounded object (if needed), followed by the phase number (if desired).

It is often a difficult problem to decide what the order of relaxation for the initial parameters should be. This must sometimes be done by trial and error. However, AD Model Builder makes the process a lot simpler. One only needs to change the phase numbers of the initial parameters in the `PARAMETER_SECTION` and recompile the program.

Often in statistical modeling, it is useful to regard a vector of quantities x_i as consisting of an overall mean, μ, and a set of deviations from that mean, δ_i, so that

$$x_i = \mu + \delta_i \qquad \text{where } \sum_i \delta_i = 0$$

AD Model Builder provides support for this modeling construction with the

```
init_bounded_dev_vector
```

declaration. The components of an object created by this declaration will automatically sum to zero without any user intervention. The line

```
init_bounded_dev_vector effort_devs(1,nobs,-5.,5.,3)
```

declares `effort_devs` to be this kind of object. The bounds `-5.,5.` control the range of the deviations. Putting reasonable bounds on such deviations often improves the stability of the estimation procedure.

AD Model Builder has `sdreport_number`, `sdreport_vector`, and `sdreport_matrix` declarations in the `PARAMETER_SECTION`. These objects behave the same as `number`, `vector`, and `matrix` objects, with the additional property that they are included in the report of the estimated standard deviations and correlation matrix.

For example, merely by including the statement `sdreport_number B_projected`, one can obtain the estimated standard deviation of the biomass projection for the next year. (Of course, you must also set `B_projected` equal to the projected biomass. This is done in the `PROCEDURE_SECTION`.)

```
PARAMETER_SECTION
  init_bounded_number q(0.,1.)
```

```
  init_bounded_number beta(0.,5.)
  init_bounded_number r(0.,5,2)
  init_number log_binit(2)
  init_bounded_dev_vector effort_devs(1,nobs,-5.,5.,3)
  init_bounded_number m(1,10.,4)
  init_bounded_vector k_devs(2,nobs,-5.,5.,4)
  number binit
  vector pred_catch(1,nobs)
  vector biomass(1,nobs)
  vector f(1,nobs)
  vector k(1,nobs)
  vector k_trend(1,nobs)
  sdreport_number k_1
  sdreport_number k_last
  sdreport_number k_change
  sdreport_number k_ratio
  sdreport_number B_projected
  number tmp_mort;
  number bio_tmp;
  number c_tmp;
  objective_function_value ff;
```

The `PRELIMINARY_CALCS_SECTION` carries out a few simple operations on the data. The model expects to have catch and effort data, but the input file contained catch and "cpue" ("catch/effort") data. We divide the catch data by the cpue data to get the effort data. The AUTODIF operation `elem_div`, which performs element-wise divisions of vector objects, is used. As usual, the same thing could have been accomplished by employing a loop and writing element-wise code. The effort data are then normalized—that is, they are divided by their average so that their average becomes 1. This is done so that we have a good idea what the catchability parameter `q` should be to give reasonable values for the fishing mortality rate (since $F = qE$).

Notice that the `PRELIMINARY_CALCS_SECTION` is C++ code, so that statements must be ended with a semicolon.

```
PRELIMINARY_CALCS_SECTION
  // get the data out of the data matrix into
  obs_catch=column(data,2);
  cpue=column(data,3);
  // divide the catch by the cpue to get the effort
  effort=elem_div(obs_catch,cpue);
  // normalize the effort and save the average
  double avg_effort=mean(effort);
  effort/=avg_effort;
```

The PROCEDURE_SECTION contains several new AD Model Builder features. Some have to do with the notion of carrying out the minimization in a number of steps or phases. The line

```
if (active(effort_devs)) f=elem_prod(f,exp(effort_devs));
```

introduces the active function. This function can be used on any initial parameter and will return a value "true" if that parameter is active in the current phase. The idea here is that if the initial parameters effort_devs are not active, then since their value is zero, carrying out the calculations will have no effect, and we can save time by avoiding the calculations. The active function is also used in the statement

```
if (!active(log_binit))
{
  log_binit=log(obs_catch(1)/(q*effort(1)));
}
```

The idea is that if the log_binit initial parameter (this is the logarithm of the biomass at the beginning of the first year) is not active, then we set it equal to the value that produces the observed catch (using the relationship $C = qEB$, such that $B = C/(qE)$. The active function is also used in the calculations of the objective function, so that unnecessary calculations are avoided.

The following code helps to deal with convergence problems in this type of nonlinear model. The problem is that the starting parameter values are often so bad that the optimization procedure will try to make the population very large and the exploitation rate very small, because this is the best local solution near the starting parameter values. To circumvent this problem, we include a penalty function to keep the average value of the fishing mortality rate f close to 0.2 during the first two phases of the minimization. In the final phase, the size of the penalty term is reduced to a very small value. The function current_phase() returns the value of the current phase of the minimization:

```
if (current_phase()<3)
 {
   ff+=1000.*square(log(mean(f)/.4));
 }
```

1.19 Using functions to improve code organization

Subroutines or functions are used to improve the organization of the code. The code for the main part of the PROCEDURE_SECTION that invokes the functions should be placed at the top of the PROCEDURE_SECTION.

```
PROCEDURE_SECTION
  // calculate the fishing mortality
  calculate_fishing_mortality();
  // calculate the biomass and predicted catch
```

```
  calculate_biomass_and_predicted_catch();
  // calculate the objective function
  calculate_the_objective_function();
```

There are three user-defined functions called at the beginning of the `PROCEDURE_SECTION`. The code to define the functions comes next. To define a function whose name is, say, `name`, the template directive `FUNCTION name` is used. Notice that no parentheses `()` are used in the definition of the function, but to call the function, the statement takes the form `name();`

1.20 A fisheries catch-at-age model

This section describes a simple catch-at-age model. The data input to this model include estimates of the numbers at age caught by the fishery each year and estimates the fishing effort each year. This example introduces AD Model Builder's ability to automatically calculate profile likelihoods for carrying out Bayesian inference. To cause the profile likelihood calculations to be carried out, use the `-lprof` command line argument.

Let i index fishing years $1 \le i \le n$ and j index age classes, with $1 \le j \le r$. The instantaneous fishing mortality rate is assumed to have the form $F_{ij} = qE_i s_j \exp(\delta_i)$, where q is called the "catchability," E_i is the observed fishing effort, s_j is an age-dependent effect termed the "selectivity," and the δ_i are deviations from the expected relationship between the observed fishing effort and the resulting fishing mortality. The δ_i are assumed to be normally distributed, with mean 0. The instantaneous natural mortality rate M is assumed to be independent of year and age class. It is not estimated in this version of the model. The instantaneous total mortality rate is given by $Z_{ij} = F_{ij} + M$. The survival rate is given by $S_{ij} = \exp(-Z_{ij})$. The number of age-class j fish in the population in year i is denoted by N_{ij}. The relationship $N_{i+1,j+1} = N_{ij}S_{ij}$ is assumed to hold. Note that using this relationship, if one knows S_{ij}, then all the N_{ij} can be calculated from knowledge of the initial population in year 1, $N_{11}, N_{12}, \ldots, N_{1r}$ and knowledge of the recruitment in each year $N_{21}, N_{31}, \ldots N_{n1}$.

The purpose of the model is to estimate quantities of interest to managers, such as the population size and exploitation rates, and to make projections about the population. In particular, we can get an estimate of the numbers of fish in the population in year $n+1$ for age classes 2 or greater from the relationship $N_{n+1,j+1} = N_{nj}S_{nj}$. If we have estimates m_j for the mean weight at age j, then the projected biomass level B_{n+1} of age class 2+ fish for year $n+1$ can be computed from the relationship $B_{n+1} = \sum_{j=2}^{r} m_j N_{n+1,j}$.

Besides getting a point estimate for quantities of interest like B_{n+1}, we also want to get an idea of how well determined the estimate is. AD Model Builder has completely automated the process of deriving good confidence limits for these parameters in a Bayesian context. One simply needs to declare the parameter to be of type `likeprof_number`. The results are given in Section 1.21.

The code for the catch-at-age model is:

```
DATA_SECTION
  // the number of years of data
```

```
  init_int nyrs
  // the number of age classes in the population
  init_int nages
  // the catch-at-age data
  init_matrix obs_catch_at_age(1,nyrs,1,nages)
  //estimates of fishing effort
  init_vector effort(1,nyrs)
  // natural mortality rate
  init_number M
  // need to have relative weight at age to calculate biomass of 2+
  vector relwt(2,nages)
INITIALIZATION_SECTION
  log_q -1
  log_P 5
PARAMETER_SECTION
  init_number log_q(1) // log of the catchability
  init_number log_P(1) // overall population scaling parameter
  init_bounded_dev_vector log_sel_coff(1,nages-1,-15.,15.,2)
  init_bounded_dev_vector log_relpop(1,nyrs+nages-1,-15.,15.,2)
  init_bounded_dev_vector effort_devs(1,nyrs,-5.,5.,3)
  vector log_sel(1,nages)
  vector log_initpop(1,nyrs+nages-1);
  matrix F(1,nyrs,1,nages) // the instantaneous fishing mortality
  matrix Z(1,nyrs,1,nages) // the instantaneous total mortality
  matrix S(1,nyrs,1,nages) // the survival rate
  matrix N(1,nyrs,1,nages) // the predicted numbers at age
  matrix C(1,nyrs,1,nages) // the predicted catch at age
  objective_function_value f
  sdreport_number avg_F
  sdreport_vector predicted_N(2,nages)
  sdreport_vector ratio_N(2,nages)
  likeprof_number pred_B
PRELIMINARY_CALCS_SECTION
  // this is just to invent some relative average
  // weight numbers
  relwt.fill_seqadd(1.,1.);
  relwt=pow(relwt,.5);
  relwt/=max(relwt);
PROCEDURE_SECTION
  // example of using FUNCTION to structure the procedure section
  get_mortality_and_survival_rates();
```

```
  get_numbers_at_age();

  get_catch_at_age();

  evaluate_the_objective_function();

FUNCTION get_mortality_and_survival_rates
  // calculate the selectivity from the sel_coffs
  for (int j=1;j<nages;j++)
  {
    log_sel(j)=log_sel_coff(j);
  }
  // the selectivity is the same for the last two age classes
  log_sel(nages)=log_sel_coff(nages-1);

  // This is the same as F(i,j)=exp(log_q)*effort(i)*exp(log_sel(j));
  F=outer_prod(mfexp(log_q)*effort,mfexp(log_sel));
  if (active(effort_devs))
  {
    for (int i=1;i<=nyrs;i++)
    {
      F(i)=F(i)*exp(effort_devs(i));
    }
  }
  // get the total mortality
  Z=F+M;
  // get the survival rate
  S=mfexp(-1.0*Z);

FUNCTION get_numbers_at_age
  log_initpop=log_relpop+log_P;
  for (int i=1;i<=nyrs;i++)
  {
    N(i,1)=mfexp(log_initpop(i));
  }
  for (int j=2;j<=nages;j++)
  {
    N(1,j)=mfexp(log_initpop(nyrs+j-1));
  }
  for (i=1;i<nyrs;i++)
  {
    for (j=1;j<nages;j++)
```

```
    {
      N(i+1,j+1)=N(i,j)*S(i,j);
    }
  }
  // calculated predicted numbers at age for next year
  for (j=1;j<nages;j++)
  {
    predicted_N(j+1)=N(nyrs,j)*S(nyrs,j);
    ratio_N(j+1)=predicted_N(j+1)/N(1,j+1);
  }
  // calculate predicted biomass for profile
  // likelihood report
  pred_B=predicted_N *relwt;

FUNCTION get_catch_at_age
  C=elem_prod(elem_div(F,Z),elem_prod(1.-S,N));

FUNCTION evaluate_the_objective_function
  // penalty functions to ''regularize '' the solution
  f+=.01*norm2(log_relpop);
  avg_F=sum(F)/double(size_count(F));
  if (last_phase())
  {
    // a very small penalty on the average fishing mortality
    f+= .001*square(log(avg_F/.2));
  }
  else
  {
    // use a large penalty during the initial phases to keep the
    // fishing mortality high
    f+= 1000.*square(log(avg_F/.2));
  }
  // errors in variables type objective function with errors in
  // the catch at age and errors in the effort fishing mortality
  // relationship
  if (active(effort_devs)
  {
    // only include the effort_devs in the objective function if
    // they are active parameters
    f+=0.5*double(size_count(C)+size_count(effort_devs))
      * log( sum(elem_div(square(C-obs_catch_at_age),.01+C))
      + 0.1*norm2(effort_devs));
```

```
  }
  else
  {
    // objective function without the effort_devs
    f+=0.5*double(size_count(C))
      * log( sum(elem_div(square(C-obs_catch_at_age),.01+C)));
  }
REPORT_SECTION
  report << "Estimated numbers of fish " << endl;
  report << N << endl;
  report << "Estimated numbers in catch " << endl;
  report << C << endl;
  report << "Observed numbers in catch " << endl;
  report << obs_catch_at_age << endl;
  report << "Estimated fishing mortality " << endl;
  report << F << endl;
```

This model employs several instances of the `init_bounded_dev_vector` type. This type consists of a vector of numbers that sum to zero—that is, they are deviations from a common mean, and are bounded. For example, the quantities `log_relpop` are used to parameterize the logarithm of the variations in year class strength of the fish population. Putting bounds on the magnitude of the deviations helps to improve the stability of the model. The bounds are from -15.0 to 15.0, which gives the estimates of relative year class strength a dynamic range of $\exp(30.0)$.

The `FUNCTION` keyword has been employed a number of times in the `PARAMETER_SECTION` to help structure the code. A function is defined simply by using the `FUNCTION` keyword followed by the name of the function.

```
  FUNCTION get_mortality_and_survival_rates
```

Don't include the parentheses or semicolon there. To use the function, simply write its name in the procedure section.

```
  get_mortality_and_survival_rates();
```

You must include the parentheses and the semicolon here.

The `REPORT_SECTION` shows how to generate a report for an AD Model Builder program. The default report generating machinery utilizes the C++ "stream formalism." You don't need to know much about streams to make a report, but a few comments are in order. The stream formalism associates a stream object with a file. In this case, the stream object associated with the AD Model Builder report file is `report`. To write an object `xxx` into the report file, you insert the line

```
  report << xxx;
```

into the `REPORT_SECTION`. If you want to skip to a new line after writing the object, you can include the stream manipulator `endl` as in

```
report << "Estimated numbers of fish " << endl;
```

Notice that the stream operations know about common C objects, such as strings, so that it is a simple matter to put comments or labels into the report file.

1.21 Bayesian inference and the profile likelihood

AD Model Builder enables one to quickly build models with large numbers of parameters. This is especially useful for employing Bayesian analysis. Traditionally, however, it has been difficult to interpret the results of analysis using such models. In a Bayesian context, the results are represented by the posterior probability distribution for the model parameters. To get exact results from the posterior distribution, it is necessary to evaluate integrals over large-dimensional spaces. This can be computationally intractable. AD Model Builder provides approximations to these integrals in the form of the profile likelihood. The profile likelihood can be used to estimate for extreme values (such as estimating a value β so that for a parameter b, the probability that $b < \beta \approx 0.10$, or the probability that $b > \beta \approx 0.10$) for any model parameter. To use this facility, simply declare the parameter of interest to be of type `likeprof_number` in the `PARAMETER_SECTION` and assign the correct value to the parameter in the `PROCEDURE_SECTION`.

The code for the catch-at-age model estimates the profile likelihood for the projected biomass of age class 2+ fish. (Age class 2+ has been used to avoid the extra problem of dealing with the uncertainty of the recruitment of age class 1 fish.) As a typical application of the method, the user of the model can estimate the probability of biomass of fish for next year being larger or smaller than a certain value. Estimates like these are obviously of great interest to managers of natural resources.

The profile likelihood report for a variable is in a file with the same name as the variable (truncated to eight letters, if necessary, with the suffix `.PLT` appended). For this example, the report is in the file `PRED_B.PLT`. Part of the file is shown here:

```
pred_B:
Profile likelihood
 -1411.23 1.1604e-09
 -1250.5 1.71005e-09
 -1154.06 2.22411e-09
  ...................    // skip some here
  ...................
 278.258 2.79633e-05
 324.632 5.28205e-05
 388.923 6.89413e-05
 453.214 8.84641e-05
 517.505 0.0001116
 581.796 0.000138412
  ...................
```

```
 ...................
1289 0.000482459
1353.29 0.000494449
1417.58 0.000503261
1481.87 0.000508715
1546.16 0.0005107
1610.45 0.000509175
1674.74 0.000504171
1739.03 0.000490788
1803.32 0.000476089
1867.61 0.000460214
1931.91 0.000443313
1996.2 0.000425539
2060.49 0.000407049
2124.78 0.000388
2189.07 0.00036855
 ...................
 ...................
4503.55 2.27712e-05
4599.98 2.00312e-05
4760.71 1.48842e-05
4921.44 1.07058e-05
5082.16 7.45383e-06
 ...................
 ...................
6528.71 6.82689e-07
6689.44 6.91085e-07
6850.17 7.3193e-07
Minimum width confidence limits:
       significance level lower bound upper bound
             0.90           572.537    3153.43
             0.95           453.214    3467.07
             0.975          347.024    3667.76

One sided confidence limits for the profile likelihood:

The probability is   0.9 that pred_B is greater than 943.214
The probability is  0.95 that pred_B is greater than 750.503
The probability is 0.975 that pred_B is greater than 602.507

The probability is   0.9 that pred_B is less than 3173.97
The probability is  0.95 that pred_B is less than 3682.75
```

```
The probability is 0.975 that pred_B is less than 4199.03
```

The file contains the probability density function and the approximate confidence limits for the the profile likelihood and the normal approximation. Since the format is the same for both, we only discuss the profile likelihood here. The first part of the report contains pairs of numbers (x_i, y_i), which consist of values of the parameter in the report (in this case, `PRED_B`) and the estimated value for the probability density associated with that parameter at the point. The probability that the parameter x lies in the interval $x_r \leq x \leq x_s$, where $x_r < x_s$, can be estimated from the sum

$$\sum_{i=r}^{s} (x_{i+1} - x_i) y_i.$$

The reports of the one and two-sided confidence limits for the parameter were produced this way. Also, a plot of y_i versus x_i gives the user an indication of what the probability distribution of the parameter looks like. (See Figure 1.5.)

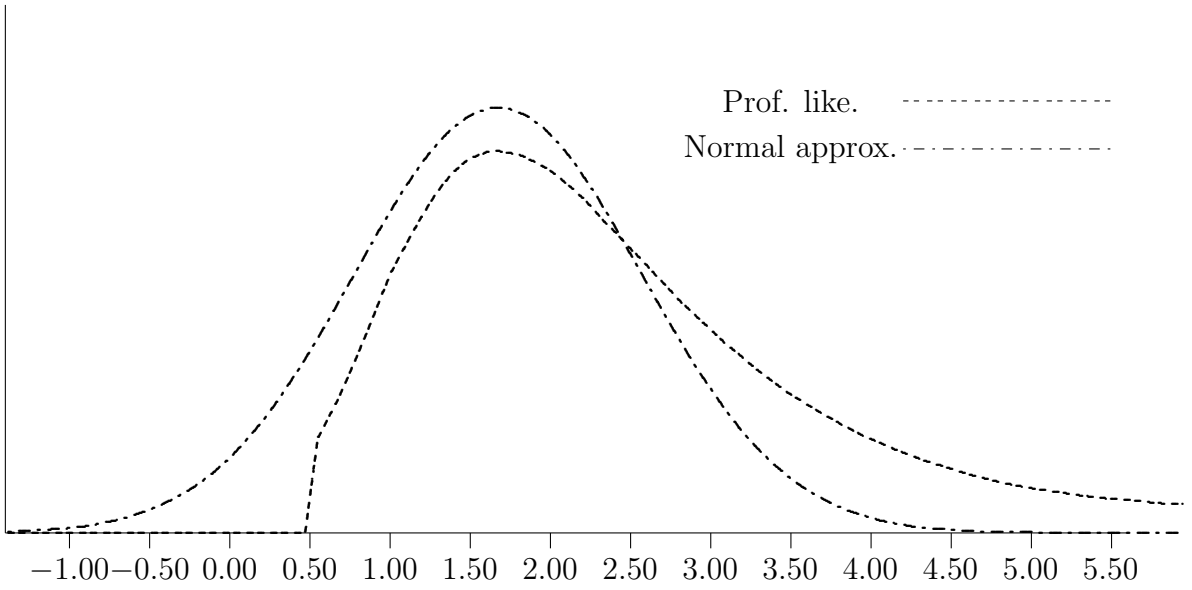


Figure 1.5: Predicted biomass of (2+) fish $\times 10^3$.

The profile likelihood indicates the fact that the biomass cannot be less than zero. The normal approximation is not very useful for calculating the probability that the biomass is very low—a question of great interest to managers, who are probably not going to be impressed by the knowledge that there is an estimated probability of 0.975 that the biomass is greater than −52.660.

```
One sided confidence limits for the normal approximation

The probability is   0.9 that pred_B is greater than 551.235
The probability is  0.95 that pred_B is greater than 202.374
```

```
The probability is 0.975 that pred_B is greater than -52.660
```

1.22 Saving the output from profile likelihood to use as starting values for MCMC analysis

If the profile likelihood calculations are carried out with the `-prsave` option, the values of the independent variables for each point on the profile are saved in a file named, say, `xxx.pvl`, where `xxx` is the name of the variable being profiled.

```
#Step -8
#num sigmas -27
 -2.96325 6.98069 -2.96893 -1.15811 0.417864 1.5352 1.50556
 0.668417 1.29106 2.04238 1.85167 1.02342 1.03264 1.35247
 1.5832 1.87033 1.67212 0.984254 -0.58013 -8.10159 0.757686
 0.958038 0.414446 -1.48443 -2.57572 -4.09184 -0.869426 -0.545055
 -0.333125 -0.350978 -0.487261 -0.123192 -0.158569 -0.434328
 -0.609651 -0.684244 -0.405214 5.00104
#Step -7
#num sigmas -22
  // ..........................
#Step 7
#num sigmas 22
 -5.94034 9.29211 -2.6122 0.0773101 1.54853 1.91895 0.578923
-1.51152 0.0124827 0.712157 0.520084 -0.202059 -0.0505122
0.284112 0.469956 0.731273 0.664325 0.642344 0.691073
-1.10233 -0.362781 0.034522 0.0127999 -0.538117 -0.575466
-1.94386 -0.544077 -0.0349702 0.349352 0.355073 0.237236
0.335559 0.177427 -0.0507647 -0.167382 -0.303103 -0.249956 -0.104393
#Step 8
#num sigmas 27
 -6.09524 9.43103 -2.59874 0.0930842 1.55938
1.91285 0.561478 -1.52804 -0.0139936 0.687758 0.502089
-0.212203 -0.0519722 0.287149 0.474422 0.739316 0.678415
0.663857 0.71933 -1.07637 -0.387684 0.0146463 0.00647923
-0.530625 -0.566471 -1.93414 -0.521944 -0.0111346 0.372352
0.372706 0.247599 0.333505 0.171122 -0.0585298 -0.177735
-0.319115 -0.273111 -0.135715
```

To use the values as a starting point for the MCMC analysis, use a text editor to put the desired starting values in a file by themselves. Suppose that the file name is `mcmc.dat`. Run the MCMC analysis with the option `-mcpin mcmc.dat` and it will begin the MCMC analysis from that file.

1.23 The profile likelihood calculations

We have been told that the profile likelihood as calculated in AD Model Builder for dependent variables may differ from that calculated by other authors. This section will clarify what we mean by the term and will motivate our calculation.

Let $(x_1, \ldots, x_n)$ be n independent variables, $f(x_1, \ldots, x_n)$ be a probability density function, and g denote a dependent variable—that is, a real valued function of $(x_1, \ldots, x_n)$. The profile likelihood calculation for g is intended to produce an approximation to the probability density function for g.

Consider first the case, where g is equal to one of the independent variables, say $g = x_1$. In this simple case, the marginal distribution of x_1 is give by the integral

$$\int f(x_1, ..., x_n)\, \mathrm{d}x_2 \mathrm{d}x_3 \cdots \mathrm{d}x_n \tag{1.15}$$

The use of the profile likelihood in this case is based on the assumption (or hope) that there exists a constant λ independent of x_1 such that $\lambda \max_{x_2,...,x_n}\{f(x_1, ..., x_n)\}$ is a good approximation to this integral.

This approach should be useful for a lot of applications based on the fact that the central limit theorem implies that for a lot of observations, the posterior probability distribution is more or less well approximated by a multivariate normal distribution, and for such distributions, the assumptions holds exactly. So the profile likelihood is calculated by calculating the conditional maximum of the likelihood function and then normalizing it so that it integrates to 1.

For an arbitrary dependent variable, the situation is a bit more complicated. A good approximation to a probability distribution should have the property of parameter invariance, that is, $Pr\{a \le x \le b\} = Pr\{h(a) \le h(x) \le h(b)\}$ for any monotonically increasing function h. To achieve the property of parameter invariance, we modify the definition of profile likelihood for dependent variables.

Fix a value g_0 for g and consider the integral

$$\int_{\{x: g_0 - \epsilon/2 \le g(x) \le g_0 + \epsilon/2\}} f(x_1, \ldots, x_n)\, \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_n$$

which is the probability that $g(x)$ has a value between $g_0 - \epsilon/2$ and $g_0 + \epsilon/2$. This probability depends on two quantities, the value of $f(x)$ and the thickness of the region being integrated over. We approximate $f(x)$ by its maximum value $\hat{x}(g) = \max_{\{x: g(x) = g_0\}}\{f(x)\}$. For the thickness, we have $g(\hat{x} + h) \approx g(\hat{x}) + \langle \nabla g(\hat{x}), h\rangle = \epsilon/2$, where h is a vector perpendicular to the level set of g at $\hat{x}$. However, ∇g is also perpendicular to the level set, so $\langle \nabla g(\hat{x}), h\rangle = \|\nabla g(\hat{x})\|\|h\|$, such that $\|h\| = \epsilon/(2\|g(\hat{x})\|)$. Thus, the integral is approximated by $\epsilon f(\hat{x})/\|\nabla g(\hat{x})\|$. Taking the derivative with respect to ϵ yields $f(\hat{x})/\|\nabla g(\hat{x})\|$, which is the profile likelihood expression for a dependent variable. For an independent variable, $\|\nabla g(\hat{x})\| = 1$, so our definition of the profile likelihood corresponds to the usual one in this case.

1.24 Modifying the profile likelihood approximation procedure

The functions `set_stepnumber()` and `set_stepsize()` can be used to modify the number of points used to approximate the profile likelihood, or to change the stepsize between the points. This can be carried out in the `PRELIMINARY_CALCS_SECTION`. If `u` has been declared to be of type `likeprof_number`,

```
PRELIMINARY_CALCS_SECTION
  u.set_stepnumber(10); // default value is 8
  u.set_stepsize(0.2);  // default value is 0.5
```

will set the number of steps equal to 21 (from -10 to 10) and will set the step size equal to 0.2 times the estimated standard deviation for the parameter `u`.

1.25 Changing the default file names for data and parameter input

The following code fragment illustrates how the files used for input of the data and parameter values can be changed. This code has been taken from the example `catage.tpl` and modified. In the `DATA_SECTION`, the data are first read in from the file `catch.dat`. Then the effort data are read in from the file `effort.dat`. The remainder of the data are read in from the file `catch.dat`. It is necessary to save the current file position in an object of type `streampos`. This object is used to position the file properly. The escape sequence `!!` can be used to include one line of the user's code into the `DATA_SECTION` or `PARAMETER_SECTION`. This is more compact than the `LOCAL_CALCS` construction.

```
DATA_SECTION
 // will read data from file catchdat.dat
 !! ad_comm::change_datafile_name("catchdat.dat");
  init_int nyrs
  init_int nages
  init_matrix obs_catch_at_age(1,nyrs,1,nages)
 // now read the effort data from the file effort.dat and save the current
 // file position in catchdat.dat in the object tmp
 !! streampos tmp = ad_comm::change_datafile_name("effort.dat");
  init_vector effort(1,nyrs)
 // now read the rest of the data from the file catchdat.dat
 // including the ioption argument tmp will reset the file to that position
 !! ad_comm::change_datafile_name("catchdat.dat",tmp);
  init_number M

 // ....
```

```
PARAMETER_SECTION
 // will read parameters from file catch.par
 !! ad_comm::change_parfile_name("catch.par");
```

1.26 Using the subvector operation to avoid writing loops

If `v` is a vector object, then for integers `l` and `u`, the expression `v(l,u)` is a vector object of the same type, with minimum valid index `l` and maximum valid index `u`. (Of course, `l` and `u` must be within the valid index range for `v`, and `l` must be less than or equal to `u`.) The subvector formed by this operation can be used on both sides of the equals sign in an arithmetic expression. The number of loops that must be written can be significantly reduced in this manner. We shall use the `subvector` operator to remove some of the loops in the catch-at-age model code.

```
  // calculate the selectivity from the sel_coffs
  for (int j=1;j<nages;j++)
  {
    log_sel(j)=log_sel_coff(j);
  }
  // the selectivity is the same for the last two age classes
  log_sel(nages)=log_sel_coff(nages-1);

  // same code using the subvector operation
  log_sel(1,nage-1)=log_sel_coff;
  // the selectivity is the same for the last two age classes
  log_sel(nages)=log_sel_coff(nages-1);
```

Notice that `log_sel(1,nage-1)` is not a distinct vector from `log_sel`. This means that an assignment to `log_sel(1,nage-1)` is an assignment to a part of `log_sel`. The next example is a bit more complicated. It involves taking a row of a matrix to form a vector, forming a subvector, and changing the valid index range for the vector.

```
  // loop form of the code
  for (i=1;i<nyrs;i++)
  {
    for (j=1;j<nages;j++)
    {
      N(i+1,j+1)=N(i,j)*S(i,j);
    }
  }

  // can only eliminate the inside loop
```

```
  for (i=1;i<nyrs;i++)
  {
    // ++ increments the index bounds by 1
    N(i+1)(2,nyrs)=++elem_prod(N(i)(1,nage-1),S(i)(1,nage-1));
  }
```

Notice that `N(i+1)` is a vector object, so `N(i+1)(2,nyrs)` is a subvector of `N(i)`. Another point is that `elem_prod(N(i)(1,nage-1),S(i)(1,nage-1))` is a vector object with minimum valid index 1 and maximum valid index `nyrs-1`. The operator `++` applied to a subvector increments the valid index range by 1, so that it has the same range of valid index values as `N(i+1)(2,nyrs)`. The operator `--@--` would decrement the valid index range by 1.

1.27 The use of higher-dimensional arrays

The example contained in the file `FOURD.TPL` illustrates some aspects of the use of 3 and 4-dimensional arrays. There are now examples of the use of arrays up to dimension 7 in the documentation. [2]

```
DATA_SECTION
  init_4darray d4(1,2,1,2,1,3,1,3)
  init_3darray d3(1,2,1,3,1,3)
PARAMETER_SECTION
  init_matrix M(1,3,1,3)
  4darray p4(1,2,1,2,1,3,2,3)
  objective_function_value f
PRELIMINARY_CALCS_SECTION
 for (int i=1;i<=3;i++)
 {
   M(i,i)=1;  // set M equal to the identity matrix to start
 }
PROCEDURE_SECTION
 for (int i=1;i<=2;i++)
 {
   for (int j=1;j<=2;j++)
   {
     // d4(i,j) is a 3x3 matrix -- d3(i) is a 3x3 matrix
     // d4(i,j)*M is matrix multiplication -- inv(M) is matrix inverse
     f+= norm2( d4(i,j)*M + d3(i)+ inv(M) );
   }
 }
REPORT_SECTION
  report << "Printout of a 4 dimensional array" << endl << endl;
```

[2] See Chapter 4 for an example of the use of higher-dimensional arrays.

```
  report << d4 << endl << endl;
  report << "Printout of a 3 dimensional array" << endl << endl;
  report << d3 << endl << endl;
```

In the DATA_SECTION, you can use 3darrays, 4darrays,..., 7darrays, and init_3darrays, init_4darrays,..., init_7darrays. In the PARAMETER_SECTION, you can use 3darrays, 4darrays,..., 7darrays, and init_3darrays, init_4darrays,..., init_5darrays, at the time of writing.

If d4 is a 4darray, then d4(i) is a 3-dimensional array and d4(i,j) is a matrix object, so d4(i,j)*M is matrix multiplication. Similarly, if d3 is a 3darray, then d3(i) is a matrix object, so d4(i,j)*M + d3(i) + inv(M) combines matrix multiplication, matrix inversion, and matrix addition.

1.28 The TOP_OF_MAIN section

The TOP_OF_MAIN section is intended to allow the programmer to insert any desired C++ code at the top of the main() function in the program. The code is copied literally from the template to the program. This section can be used to set the AUTODIF global variables. (See the AUTODIF user's manual chapter on AUTODIF global variables.) The following code fragment will set these variables:

```
TOP_OF_MAIN_SECTION
  arrmblsize = 200000; // use instead of
                  // gradient_structure::set_ARRAY_MEMBLOCK_SIZE
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(100000); // this may be
                                      // incorrect in the AUTODIF manual.
  gradient_structure::set_CMPDIF_BUFFER_SIZE(50000);
  gradient_structure::set_MAX_NVAR_OFFSET(500); // can have up to 500
                                          // independent variables
  gradient_structure::set_MAX_NUM_DEPENDENT_VARIABLES(500); // can have
                                        // up to 500 dependent variables
```

Note that within AD Model Builder, one doesn't use the function

```
  gradient_structure::set_ARRAY_MEMBLOCK_SIZE
```

to set the amount of memory available for variable arrays. Instead, use the line of code

```
  arrmblsize = nnn;
```

where nnn is the amount of memory desired.

1.29 The GLOBALS_SECTION

The GLOBALS_SECTION is intended to allow the programmer to insert any desired C++ code before the main() function in the program. The code is copied literally from the template to

the program. This enables the programmer to define global objects, and to include include header files and user-defined functions into the generated C++ code.

1.30 The BETWEEN_PHASES_SECTION

Code in `BETWEEN_PHASES_SECTION` is executed before each phase of the minimization. It is possible to carry out different actions that depend on what phase of the minimization is to begin, by using a `switch` statement (you can read about this in a book on C or C++), together with the `current_phase()` function.

```
switch (current_phase())
{
case 1:
  // some action
  cout << "Before phase 1 minimization " << endl;
  break;
case 2: i
  // some action
  cout << "Before phase 2 minimization " << endl;
  break;
// ....
}
```

Chapter 2

Markov Chain Simulation

2.1 Introduction to the Markov Chain Monte Carlo Approach in Bayesian Analysis

The reference for this chapter is [3], Chapter 11).

The Markov chain Monte Carlo method (MCMC) is a method for approximating the posterior distribution for parameters of interest in the Bayesian framework. This option is invoked by using the command line option `-mcmc N`, where `N` is the number of simulations performed. You will probably also want to include the option `-mcscale`, which dynamically scales the covariance matrix until a reasonable acceptance rate is observed. You may also want to use the `-mcmult n` option, which scales the initial covariances matrix if the initial values are so large that arithmetic errors occur. One advantage of AD Model Builder over some other implementations of MCMC is that the mode of the posterior distribution, together with the Hessian at the mode, is available to use for the MCMC routine. This information is used to implement a version of the Hastings-Metropolis algorithm. Another advantage is that with AD Model Builder, it is possible to calculate the profile likelihood for a parameter of interest and compare the distribution to the MCMC distribution for that parameter. A large discrepancy may indicate that one or both estimates are inadequate. If you wish to do more simulations (and to carry on from where the last one ended), use the `-mcr` option. Figure 2.1 compares the profile likelihood for the projected biomass to the estimates produced by the MCMC method, for different sample sizes (25,000 and 2,500,000 samples) for the `catage` example.

A report containing the observed distributions is produced in the file `root.hst`. All objects of type `sdreport`, i.e., `number`, `vector`, or `matrix`, are included. It is possible to save the results of every $\mathtt{n}^{\text{th}}$ simulation by using the `-mcsave n` option. Afterwords, these values can be used by running the model with the `-mceval` option, which will evaluate the `userfunction` once for every saved simulation value. At this time, the function `mceval_phase()` will return the value "true," and can be used as a switch to perform desired calculations. The results are saved in a binary file `root.psv`. If you want to convert this file into ASCII, see the next section. If you have a large number of variables of type `sdreport`,

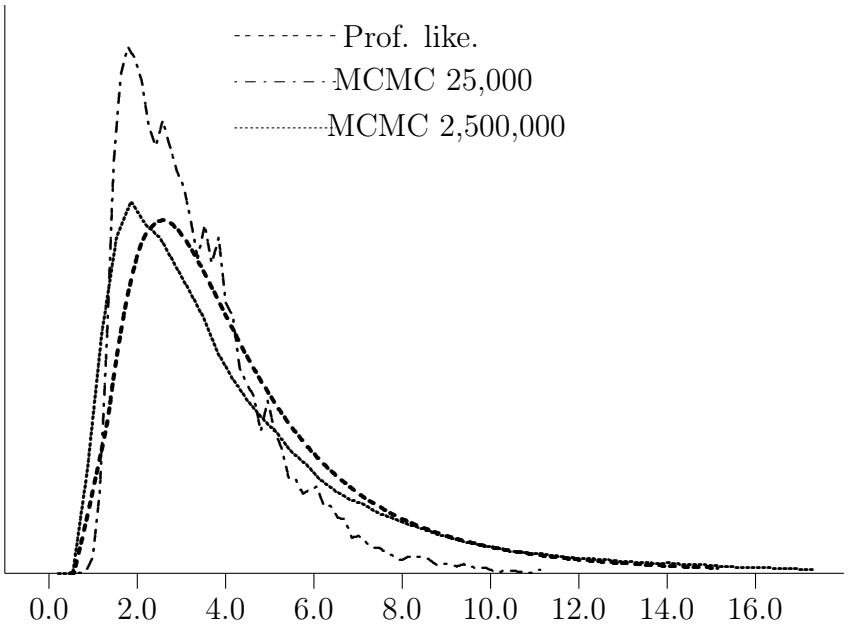


Figure 2.1: Predicted biomass of (2+) fish $\times 10^3$.

calculating the values of them for the MCMC can appreciably slow down the calculations. To turn off these calculations during the `-mcsave` phase, use the option `-nosdmcmc`. *Note: If you use this option and restart the* `mcmc` *calculations with the* `-mcr` *option, you must use the* `-nosdmcmc` *as well. Otherwise, the program will try to read in the non-existent histogram data.*

AD Model Builder uses the Hessian to produce an (almost) multivariate normal distribution for the Metropolis-Hastings algorithm. It is not exactly multivariate normal, because the random vectors produced are modified to satisfy any bounds on the parameters.

There is also an option for using a fatter-tailed distribution. This distribution is a mixture of the multivariate normal and a fat-tailed distribution. It is invoked with the `-mcprobe n` option, where `n` is the amount of fat-tailed distribution in the mixture. Probably, a value of `n` between 0.05 and 0.10 is best.

2.2 Reading AD Model Builder binary files

Often, the data that AD Model Builder needs to save are saved in the form of a binary file, using the `uistream` and `uostream` classes. If these data consist of a series of vectors, all of which have the same dimension, they are often saved in this form, where the dimension is saved at the top of the file, and the vectors are saved afterwards. It may be useful to convert these numbers into binary form, so they can be put into other programs, such as spreadsheets. The following code will read the contents of these binary files. You should call the program `readbin.cpp`. It should be a simple matter to modify this program for other uses.

```
#include <fvar.hpp>
/*  program to read a binary file (using ADMB's uistream and
    uostream stream classes) of vectors of length n.
    It is assumed that the size n is stored at the top of
    the file. there is no information about any many vectors
    are stored so we must check for an eof after each read
    To use the program you type:

                readbin filename
*/
void produce_comma_delimited_output(dvector& v)
{
  int i1=v.indexmin();
  int i2=v.indexmax();
  for (int i=i1;i<=i2;i++)
  {
    cout << v(i) << ",";
  }
  cout << endl;
}

main(int argc, char * argv[])
{
  if (argc < 2)
  {
    cerr << " Usage: progname inputfilename" << endl;
    exit(1);
  }
  uistream uis = uistream(argv[1]);
  if (!uis)
  {
    cerr << " Error trying to open binary input file "
         <<  argv[1] << endl;
    exit(1);
  }
  int ndim;
  uis >> ndim;
  if (!uis)
  {
    cerr << " Error trying to read dimension of the vector"
           " from the top of the file "
         <<  argv[1] << endl;
```

```
  exit(1);
}
if (ndim <=0)
{
  cerr << " Read invalid dimension for the vector"
         " from the top of the file "
       <<  argv[1] << " the number was " << ndim << endl;
  exit(1);
}

int nswitch;
cout << " 1 to see all records" << endl
     << " 2 then after the prompts n1 and n2 to see all" << endl
     << " records between n1 and n2 inclusive" << endl
     << " 3 to see the dimension of the vector" << endl
     << " 4 to see how many vectors there are" << endl;
cin >> nswitch;
dvector rec(1,ndim);
int n1=0;
int n2=0;
int ii=0;
switch(nswitch)
{
case 2:
  cout << " Put in the number for the first record you want to see"
       << endl;
  cin >> n1;
  cout << " Put in the number for the second record you want to see"
       << endl;
  cin >> n2;
case 1:
  do
  {
    uis >> rec;
    if  (uis.eof()) break;
    if (!uis)
    {
      cerr << " Error trying to read vector number " << ii
           << " from file " << argv[1] << endl;
      exit(1);
    }
    ii++;
```

```
      if (!n1)
      {
        // comment out the one you don't want
        //cout << rec << endl;
        produce_comma_delimited_output(rec);
      }
      else
      {
        if (n1<=ii && ii<=n2)
        {
          // comment out the one you don't want
          //cout << rec << endl;
          produce_comma_delimited_output(rec);
        }
      }
    }
    while (1);
    break;
  case 4:
    do
    {
      uis >> rec;
      if  (uis.eof()) break;
      if (!uis)
      {
        cerr << " Error trying to read vector number " << ii
             << " from file " << argv[1] << endl;
        exit(1);
      }
      ii++;
    }
    while (1);
    cout << " There are " << ii << " vectors" << endl;
    break;
  case 3:
    cout << " Dimension = " << ndim << endl;
  default:
    ;
  }
}
```

2.3 Convergence diagnostics for MCMC analysis

A major difficulty with MCMC analysis is determining whether or not the chain has converged to the underlying distribution. In general, it is never possible to prove that this convergence has occurred. In this section, we concentrate on methods that hopefully will detect situations when convergence has not occurred.

The default MCMC method employed in AD Model Builder takes advantage of the fact that AD Model Builder can find the mode of the posterior distribution and compute the Hessian at the mode. If the posterior distribution is well approximated by a multivariate normal centered at the mode, with covariance matrix equal to the inverse of the Hessian, this method can be extremely efficient for many parameter problems—especially when compared to simpler methods, such as the Gibbs sampler. The price one pays for this increased efficiency is that the method is not as robust as is the Gibbs sampler, and for some problems, it will perform much more poorly than does the Gibbs sampler.

As an example of this poor performance, we consider a simple three-parameter model developed by Vivian Haist to analyze Bowhead whale data.

The data for the model consist of total catches between 1848 and 1993, together with an estimate of the biomass in 1988, and an estimate of the change in relative biomass between 1978 and 1988.

```
DATA_SECTION
  init_vector cat(1848,1993)

PARAMETER_SECTION
  init_bounded_number k(5000,40000,1)
  init_bounded_number r(0,0.10,1)
  init_bounded_number p(0.5,1,2)
  number delta;
  vector bio(1848,1994);
  likeprof_number fink
 !! fink.set_stepsize(.003);
 !! fink.set_stepnumber(20);
  sdreport_number finr
  sdreport_number finp
  objective_function_value f
PROCEDURE_SECTION
  if (initial_params::mc_phase)
  {
    cout << k << endl;
    cout << r << endl;
    cout << p << endl;
  }
  bio(1848)=k*p;
```

```
  for (int iy=1848; iy<=1993; iy++)
  {
     dvariable fpen1=0.0;
     bio(iy+1)=posfun(bio(iy)+r*bio(iy)*(1.-(bio(iy)/k)),100.0,fpen1);
     dvariable sr=1.- cat(iy)/bio(iy);
     dvariable kcat=cat(iy);
      f+=1000*fpen1;
     if(sr< 0.05)
     {
       dvariable fpen=0.;
       kcat=bio(iy)*posfun(sr,0.05,fpen);
       f+=10000*fpen;
//     cout << " kludge "<<iy <<" "<<kcat<<" "<<cat(iy)<<" "<<fpen<<endl;
     }
     bio(iy+1)-=kcat;
  }
  finr=r;
  fink=k;
  finp=p;
  delta=(bio(1988)-bio(1978))/bio(1978);
  f+=log(sqrt(2.*PI)*500)+square(bio(1988)-7635.)/(2.*square(500));
  f+=log(sqrt(2.*PI)*.03)+square(delta-0.15)/(2.*square(.03));
```

This is a biomass dynamic model, where the biomass is assumed to satisfy the difference equation

$$B_{i+1} = B_i + r * B_i(1 - B_i/k) - C_i \tag{2.1}$$

For this formulation, there is no guarantee that the biomass will remain positive, so the `posfun` function has been used in the program to ensure that this condition will hold. This is a very "data-poor" design.

The model was fit to the data and the standard MCMC analysis was performed for it. The results were compared to an MCMC analysis performed with the Gibbs sampler. It was found that the Gibbs sampler performed better.

It is not difficult to determine why the MCMC performed so poorly. The estimated covariance matrix for the parameters is shown below. To four significant figures, the correlation between r and k is -1.0000. Thus, the Hessian matrix is almost singular.

```
  index  name   value     std.dev    1      2      3
    1    k     1.0404e+04 8.8390e+05 1.0000
    2    r     4.8838e-02 9.0337e+00 -1.0000 1.0000
    3    p     5.7293e-01 3.6946e+00 0.9998 -0.9998 1.0000
```

If the posterior distribution were exactly normally distributed, then the Hessian would be constant, i.e., not depend on the point at which is is calculated, and its use would produce

the most efficient MCMC procedure. However, in nonlinear models, the posterior distribution is not normally distributed, so the Hessian changes as we move away from the mode. Using an almost singular Hessian can make things perform very badly, as in the present case.

To deal with almost singular Hessians, we have added the `-mcrb N` option. This option reduces the amount of correlation in the Hessian, while leaving the standard deviations fixed. The number `N` should be between 1 and 9. The smaller the number, the more the correlation is reduced. For this example (see Figure 2.2), a value of 3 seemed to perform well.

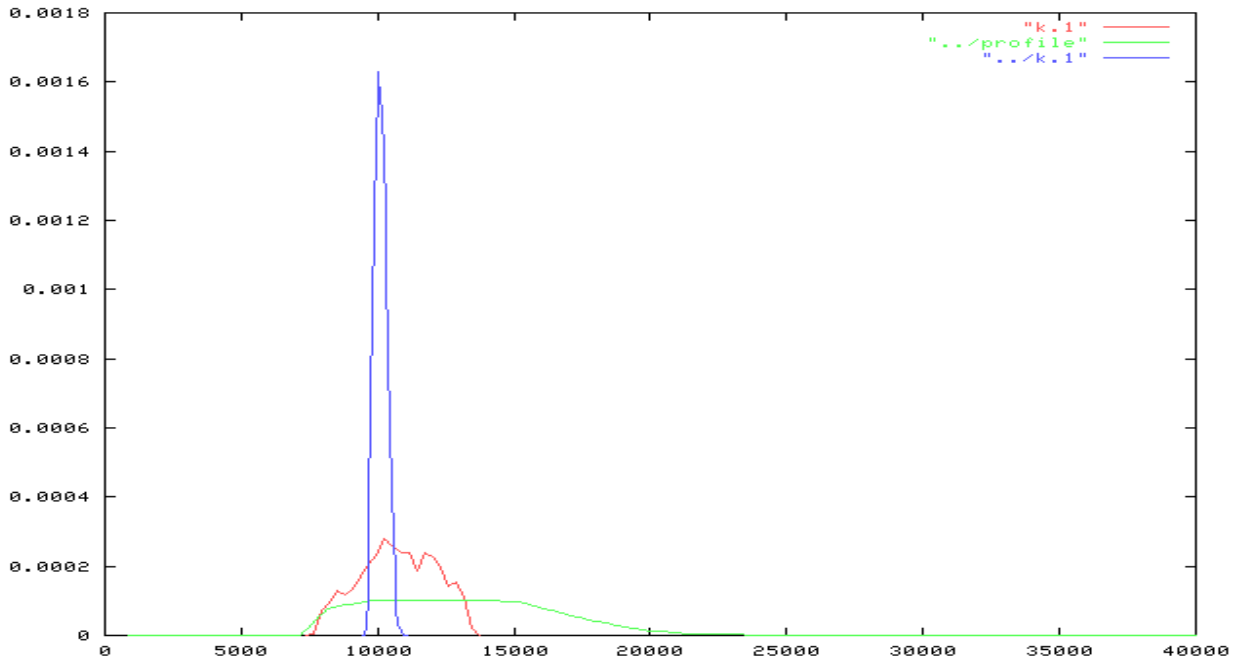


Figure 2.2

Chapter 3

A Forestry Model: Estimating the Size Distribution of Wildfires

3.1 Model description

This examples highlights two features of AD Model Builder: 1) the use of a numerical integration routine within a statistical parameter estimation model, and 2) the use of the `ad_begin_funnel` mechanism to reduce the size of temporary file storage required. It also provides a performance comparison between AD Model Builder and Splus.

This problem investigates a model that predicts a relationship between the size and frequency of wildfires. It is assumed that the probability of observing a wildfire in size category i is given by P_i, where

$$\log(P_i) = \ln\left(S_i - S_{i+1}\right) - \ln\Big(S(1)\Big).$$

If f_i is the number of wildfires observed to lie in size category i, the log-likelihood function for the problem is given by

$$l(\tau, \nu, \beta, \sigma) = \sum_i f_i \Big[\ln\left(S_i - S_{i+1}\right) - \ln\left(S(1)\right)\Big] \tag{3.1}$$

where S_i is defined by the integral

$$S_i = \int_{-\infty}^{\infty} \exp\Big\{-z^2/2 + \tau\Big(-1 + \exp\left(-\nu a_i^{\beta} \exp(\sigma z)\right)\Big)\Big\}\,\mathrm{d}z \tag{3.2}$$

The parameters τ, ν, β, and σ are functions of the parameters of the original model, and don't have a simple interpretation. Fitting the model to data involves maximizing the above log-likelihood (3.1). While the gradient can be calculated (in integral form), coding it is cumbersome. Numerically maximizing the log-likelihood without specifying the gradient is preferable.

The parameter β is related to the fractal dimension of the perimeter of the fire. One hypothesis of interest is that $\beta = 2/3$, which is related to hypotheses about the nature of the mechanism by which fires spread. The AD Model Builder code for the model follows.

```
DATA_SECTION
 int time0
 init_int nsteps
 init_int k
 init_vector a(1,k+1)
 init_vector freq(1,k)
 int a_index;
 number sum_freq
!! sum_freq=sum(freq);
PARAMETER_SECTION
  init_number log_tau
  init_number log_nu
  init_number log_beta(2)
  init_number log_sigma
  sdreport_number tau
  sdreport_number nu
  sdreport_number sigma
  sdreport_number beta
  vector S(1,k+1)
  objective_function_value f
INITIALIZATION_SECTION
  log_tau 0
  log_beta -.405465
  log_nu 0
  log_sigma -2
PROCEDURE_SECTION
  tau=exp(log_tau);
  nu=exp(log_nu);
  sigma=exp(log_sigma);
  beta=exp(log_beta);
   funnel_dvariable Integral;
   int i;
   for (i=1;i<=k+1;i++)
   {
     a_index=i;
     ad_begin_funnel();
     Integral=adromb(&model_parameters::h,-3.0,3.0,nsteps);
     S(i)=Integral;
   }
   f=0.0;
   for (i=1;i<=k;i++)
   {
```

```
    dvariable ff=0.0;
    // make the model stable for case when S(i)<=S(i+1)
    // we have to subtract s(i+1) from S(i) first or roundoff will
    // do away with the 1.e-50.
    f-=freq(i)*log(1.e-50+(S(i)-S(i+1)));
    f+=ff;
   }
   f+=sum_freq*log(1.e-50+S(1));
FUNCTION dvariable h(const dvariable& z)
  dvariable tmp;
  tmp=exp(-.5*z*z + tau*(-1.+exp(-nu*pow(a(a_index),beta)*exp(sigma*z))) );
  return tmp;
REPORT_SECTION
  int * pt=NULL;
  report << " elapsed time = " << time(pt)-time0 << " seconds" << endl;
  report << "nsteps = " << setprecision(10) << nsteps << endl;
  report << "f = " << setprecision(10) << f << endl;
  report << "a" << endl << a << endl;
  report << "freq" << endl << freq << endl;
  report << "S" << endl << S << endl;
  report << "S/S(1)" << endl << setfixed << setprecision(6) << S/S(1) << endl;
  report << "tau " << tau << endl;
  report << "nu " << nu << endl;
  report << "beta " << beta << endl;
  report << "sigma " << sigma << endl;
```

3.2 The numerical integration routine

The statement

```
Integral=adromb(&model_parameters::h,-3.0,3.0,nsteps);
```

invokes the numerical integration routine for the user-defined function `h`. The function must be defined in a `FUNCTION` subsection. It can have any name, must be defined to take a `const dvariable&` argument, and must return a `dvariable`. The values -3.0 and 3.0 are the limits of integration (effectively $-\infty$, ∞ for this example). The integer argument `nsteps` determines how accurate the integration will be. Higher values of `nsteps` will be more accurate, but greatly increase the amount of time necessary to fit the model. The basic strategy is to use a moderate value for `nsteps`, such as 6, and then to increase this value to see if the parameter estimates change much.

```
FUNCTION dvariable h(const dvariable& z)
```

3.3 Using the ad_begin_funnel routine to reduce the amount of temporary storage required

Numerical integration routines can be very computationally intensive, especially when they must be computed to great accuracy. Such computations will require a lot of temporary storage in AD Model Builder. Fortunately, the output from such a routine is just one number: the value of the integral. In automatic differentiation terminology, a long set of computations that produce just one number is known as a "funnel." It is possible to exploit the properties of such a funnel to greatly reduce the amount of temporary storage required. All that is necessary is to declare an object of type `funnel_dvariable` and to assign the results of the computation to it. At the beginning of the funnel, a call to the function `ad_begin_funnel` is made. There is quite a bit of overhead associated with the funnel construction, so it should not be used for very small calculations. However, it is possible to put it in and test the program to see whether or not it runs more quickly. The following modified code will produce exactly the same results, but without the funnel construction:

```
dvariable Integral; // change the definition of Integral
int i;
for (i=1;i<=k+1;i++)
{
  a_index=i;
  // ad_begin_funnel(); // comment out this line
  Integral=adromb(&model_parameters::h,-3.0,3.0,nsteps);
  S(i)=Integral;
}
```

If the funnel construction is used on a portion of code that is not a funnel, incorrect derivative values will be obtained. If this is suspected, the funnel should be removed, as in the above example, and the model run again.

3.4 Effect of the accuracy switch on the running time for numerical integration

The following report shows the amount of time required to run the model with a fixed value of β for different values of the parameter `nsteps`. For practical purposes, a value of `nsteps=8` gives enough accuracy so that the model could be fit in about 6 seconds.

```
elapsed time = 2 seconds nsteps = 6 f = 629.9846518
tau 9.851110 nu 8.913479 beta 0.666667 sigma 1.885570

elapsed time = 2 seconds nsteps = 7 f = 629.9851092
tau 9.850213 nu 8.835066 beta 0.666667 sigma 1.882967
```

```
elapsed time = 6 seconds nsteps = 8 f = 629.9851223
tau 9.850227 nu 8.836769 beta 0.666667 sigma 1.883024

elapsed time = 6 seconds nsteps = 9 f = 629.9851222
tau 9.850226 nu 8.836769 beta 0.666667 sigma 1.883024

elapsed time = 14 seconds nsteps = 10 f = 629.9851222
tau 9.850226 nu 8.836769 beta 0.666667 sigma 1.883024
```

The corresponding times when `beta` was estimated in an extra phase of the minimization are given here. It as apparent that the model parameters become unstable when beta is being estimated. Twice the log-likelihood difference is $2(629.98 - 627.31) = 5.34$ which is significant.

```
elapsed time = 3 seconds nsteps = 6 f = 627.2919906
tau 20.729183 nu 427.816375 beta 0.180225 sigma 2.499445

elapsed time = 6 seconds nsteps = 7 f = 627.2952716
tau 21.868971 nu 80914.970724 beta 0.170392 sigma 4.232237

elapsed time = 17 seconds nsteps = 8 f = 627.297021
tau 22.858629 nu 2326271883.421848 beta 0.164749 sigma 7.653068

elapsed time = 62 seconds nsteps = 9 f = 627.2993787
tau 23.771061 nu 1652877622661391616.000000 beta 0.161073 sigma 14.451510

elapsed time = 123 seconds nsteps = 10 f = 627.3106333
tau 23.116097 nu 49753858778.636856 beta 0.159364 sigma 8.663666

elapsed time = 244 seconds nsteps = 11 f = 627.310624
tau 23.115275 nu 49009470510.133156 beta 0.159369 sigma 8.658643
```

3.5 A comparison with Splus for the forestry model

The Splus minimizing routine `nlminb` was used to fit the model. Fitting the three-parameter model with Splus required approximately 280 seconds, compared to 6 seconds with AD Model Builder, so that AD Model Builder was approximately 45 times faster for this simple problem.

For the four parameter problem with beta estimated, the SPLUS routine exited after 14 minutes and 30 seconds, reporting false convergence with a function value of 627.338.

The data for the example is

```
a
 0.04 0.1 0.2 0.4 0.8 1.6 3.2 6.4 12.8 25.6 51.2 102.4 204.8
```

```
freq
 167 84 61 29 19 17 4 4 1 0 1 1
```

where the first line contains the bounds for the size categories and the second line contains the number of observations in each size category. The Splus code with fixed beta for the example is

```
obj.20<-
function(xvec)
{
#Objective for maxn in NLMINB NB vector argument
 - llik.20(xvec[1], xvec[2], xvec[3])
}
llik.20<-
function(logtau, lognu, logsigma)
{
        tau<-exp(logtau)
        nu<-exp(lognu)
        sigma<-exp(logsigma)
        print(tau)
        print(nu)
        print(sigma)
        llik <- 0
        for(i in 1:(length(freq)+1)) {
           Int[i]<-S.20(xa[i], tau, nu, sigma)
        }
        print(llik)
        for(i in 1:length(freq)) {
           llik <- llik + (freq[i] * (log(1.e-50+(Int[i]-Int[i+1]))
               -log(1.e-50+Int[1])))
        }
        llik
}
S.20<-
function(da, tau, nu, sigma)
{
        results <- integrate(intgnd.20, -3, 3, TAU = tau, NU = nu, SIGMA =
                sigma, A = da)
        if(results\$message != "normal termination")
                ans <- results\$message
        else ans <- results\$integral
        ans
}
intgnd.20<-
```

```
function(z, A, TAU, NU, SIGMA)
{
  exp(-0.5 * z^2 + TAU * (-1 + exp(-NU * A^2/3 * exp(SIGMA * z))))
}
```

To run the example in Splus with the same initial values, use the following values

```
  logtau 0 lognu 0 logsigma -2
```

The vector `a` should contain the 13 `a` values, while the vector `freq` should contain the 12 observed frequencies.

Chapter 4

Economic Models: Regime Switching

An active field in macroeconomic modeling is the area of "regime switching." This is discussed in greater generality in [5], Chapter 22. The code for the following example is based on the domain switching model taken from [4]. This example is not ideal for exploiting AD Model Builder's greatest advantage, which is the ability to estimate parameters in models with a large number of independent variables. However, it does illustrate the efficacy of the use of higher (up to 7-dimensional) arrays in AD Model Builder.

4.1 Analysis of economic data from [4]

For this model, the observed quantities are the Y_t, where

$$Y_t = a_0 + a_1 s_{ti} + Z_t \tag{4.1}$$

and the state variables Z_t satisfy the fourth-order autoregressive relationship

$$Z_t = f_1 Z_{t-1} + f_2 Z_{t-2} + f_3 Z_{t-3} + f_4 Z_{t-4} + \epsilon_t \tag{4.2}$$

where, in turn, the ϵ_t are independent, normally distributed random variables, with mean 0 and standard deviation σ. These equations correspond to Hamilton's [4] equations 4.3. The state variable s_{ti} is the realized value of a Markov process, S_t, whose evolution is described below. This coefficient takes on the value i when the system is in state i. In the current example, there are two states, so s_t takes on one of the two values 0 or 1. We can solve equation (4.1) for the values of Z_t conditioned on the unknown value of the state at time t. Let z_{ti} be defined by

$$\begin{aligned} z_{i0} &= Y_t - a_0 \\ z_{t1} &= Y_t - a_0 - a_1 \end{aligned}$$

Let (i, j, k, l, m) be a quintuplet of state values for the states at time $t, t-1, \ldots, t-4$. Define $e(t, i, j, k, l, m)$, the realized values of the random variables ϵ_t, by

$$e(t, i, j, k, l, m) = Y_{ti} - f_1 z_{t-1,j} - f_2 z_{t-2,k} - f_3 z_{t-3,l} - f_4 z_{t-4,m}$$

Notice that due to the lags, we can only begin to calculate values for the $e(t,i,j,k,l,m)$ in time period 5. It is assumed that the state transitions are given by a Markov process with transition matrix $P = (p_{ij})$.[1] If we are in state j at time t, the probability of being in state i at time $t+1$ is p_{ij}.

If we consider the quintuple of the last 5 states to be the states of a new Markov process, then we can define the transition matrix for this process by

$$(i,j,k,l,m) \Rightarrow (0,i,j,k,l) \quad \text{with probability } p_{0i}$$

and

$$(i,j,k,l,m) \Rightarrow (1,i,j,k,l) \quad \text{with probability } p_{1i}$$

If $q(t-1,j,k,l,m,n)$ is the probability of being in state (j,k,l,m,n) at period $t-1$, the probability of being in state $q(t,i,j,k,l,m)$ at time period t is given by

$$q(t,i,j,l,,m) = \sum_n P_{ij} q(t-1,j,k,l,m,n)$$

In particular, if

$$q_b(t,i,j,k,l,m)$$

is the probability of being in the state (i,j,l,m,n) before observing Y_t, and $q_a(t-1,j,k,l,m,n)$ is the probability of being in the state (j,k,l,m,n) after observing Y_{t-1}, then

$$q_b(t,i,j,k,l,m) = \sum_n P_{ij} q_a(t-1j,k,l,m,n) \tag{4.3}$$

Let $Q(Y_t|(i,j,k,l,m),Y_{t-1},Y_{t-2},Y_{t-3},Y_{t-4})$ be the conditional probability (or probability density) for Y_t given $S_t = i, S_{t-1} = j, S_{t-2} = k, S_{t-3} = l, S_{t-4} = m, Y_{t-1}, Y_{t-2}, Y_{t-3}, Y_{t-4}$. Then, ignoring a constant term that is irrelevant for the calculations,

$$Q(Y_t|(i,j,k,l,m),Y_{t-1},Y_{t-2},Y_{t-3},Y_{t-4}) = \exp\big(-e(i,j,k,l,m)^2/2\sigma^2\big)/\sigma \tag{4.4}$$

Define $u(Y_t,i,j,k,l,m)$ by

$$u(Y_t,i,j,k,l,m) = Q(Y_t|(i,j,k,l,m),Y_{t-1},\ldots,Y_{t-4}) q_b(t,i,j,k,l,m) \tag{4.5}$$

Then, $q_a(t,i_t,j,k,l,m)$ can be calculated from the relationship

$$q_a(t,i_t,j,k,l,m) = u(Y_t,i,j,k,l,m) \Big/ \sum_{i,j,k,l,m} u(Y_t,i,j,k,l,m) \tag{4.6}$$

The log-likelihood function for the parameters can be calculated from the $u(Y_t,i,j,k,l,m)$. It is equal to

$$\sum_t \log\left(\sum_{i,j,k,l,m} u(Y_t,i,j,k,l,m)\right) \tag{4.7}$$

[1] Hamilton seems to index his matrices with the column index first in some cases. We use the row index first. Thus, Hamilton's p_{ij} may correspond to our p_{ji}.

4.2 The code for Hamilton's fourth-order autoregressive model

The complete AD Model Builder template (TPL) code is in the file `ham4.tpl`. The C++ (CPP) code produced from this is in the file `ham4.cpp`. Here is the TPL code, split up with comments:

```
DATA_SECTION
  init_number a1init // read in the initial value of a1 with the data
  init_int nperiods1 // the number of observations
  int nperiods // nperiods-1 after differencing
 !! nperiods=nperiods1-1;
  init_vector yraw(1,nperiods1) //read in the observations
  vector y(1,nperiods) // the differenced observations
 !! y=100.*(--log(yraw(2,nperiods1)) - log(yraw(1,nperiods)));
  int order
  int op1
 !! order=4; //order of the autoregressive process
 !! op1=order+1;
  int nstates // the number of states (expansion and contraction)
 !! nstates=2;
```

The `DATA_SECTION` contains constant quantities, or "data." This is in contrast to quantities that depend on parameters being estimated, which go into the `PARAMETER_SECTION`. All quantities in the `PARAMETER_SECTION` with the `init_` prefix are initial data, which must be read in from somewhere. By default, they are read in from the file `ROOT.dat` (DAT file), where "`ROOT`" is the root part of the name of the program being run (in this case, `ham4.exe`, so it is `ham4.dat`).

The first quantity is a number, `a1init`, which will be used for initializing the value of `a1` in the program. This is a simple way to try different initial values for `a1` simply by modifying the input data file. Such procedures are often valuable, to ensure that the correct global value of the objective function has been found. The second quantity, `nperiods1`, is the number of data points in the file. Notice that as soon as a quantity has been defined, it is available to use for defining other quantities. The quantity `nperiod` does not have an `init_` before it, so it will not be read in and must be calculated in terms of other quantities at some point. Since we want it now, it is calculated immediately.

```
 !! nperiods=nperiods1-1;
```

The `!!` are used to insert any valid C++ code into the `DATA_SECTION` or `PARAMETER_SECTION`. This code will be executed verbatim (after the `!!` have been stripped off, of course) at the appropriate time. The `init_vector yraw` is defined and given a size, with indices going from `1` to `nperiods1`. The `nperiods1` data points will be read into `yraw` from the DAT file. The data are immediately transformed and the resulting `nperiods` data points are put into `y`.

```
PARAMETER_SECTION
  init_vector f(1,order,1) // coefficients for the autoregressive
                           // process
  init_bounded_matrix Pcoff(0,nstates-1,0,nstates-1,.01,.99,2)
       // determines the transition matrix for the markov process
  init_number a0(5) // equation 4.3 in Hamilton (1989)
  init_bounded_number a1(0.0,10.0,4);
 !! if (a0==0.0) a1=a1init; // set initial value for a1 as specified
                    // in the top of the file nham4.dat
  init_bounded_number smult(0.01,1,3) // used in computing sigma
  matrix z(1,nperiods,0,1) // computed via equation 4.3 in
                         // Hamilton (1989)
  matrix qbefore(op1,nperiods,0,1); // prob. of being in state before
  matrix qafter(op1,nperiods,0,1); // and after observing y(t)
  number sigma // variance of epsilon(t) in equation 4.3
  number var // square of sigma
  sdreport_matrix P(0,nstates-1,0,nstates-1);
  number ff1;
  vector qb1(0,1);
  matrix qb2(0,1,0,1);
  3darray qb3(0,1,0,1,0,1);
  4darray qb4(0,1,0,1,0,1,0,1);
  6darray qb(op1,nperiods,0,1,0,1,0,1,0,1,0,1);
  6darray qa(op1,nperiods,0,1,0,1,0,1,0,1,0,1);
  6darray eps(op1,nperiods,0,1,0,1,0,1,0,1,0,1);
  6darray eps2(op1,nperiods,0,1,0,1,0,1,0,1,0,1);
  6darray prob(op1,nperiods,0,1,0,1,0,1,0,1,0,1);
  objective_function_value ff;
```

The `PARAMETER_SECTION` describes the parameters of the model, that is, the quantities to be estimated. Quantities that have the prefix `init_` are akin to the independent variables from which the log-likelihood function (or, more generally, any objective function) can be calculated. Other objects are dependent variables that must be calculated from the independent variables. The default behavior of AD Model Builder is to read in initial parameter values for the parameters from a `PAR` file, if it finds one. Otherwise, they are given default values consistent with their type. The quantity `f` is a vector of four coefficients for the autoregressive process. `Pcoff` is a 2×2 matrix used to parameterize the transition matrix `P` for the Markov process. Its values are restricted to lie between 0.01 and 0.99. `smult` is a number used to parameterize `sigma` and `var` (which is the variance) as a multiple of the mean-squared residuals. This reparameterization undimensionalizes the calculation and is a good technique to employ for nonlinear modeling in general. The transition matrix `P` is defined to be of type `sdreport_matrix`, so the standard deviation estimates for its members will be included in the standard deviation report contained in the STD file. To date, AD Model Builder sports

up to 7-dimensional arrays. For historical reasons, 1 and 2-dimensional arrays are referred to as `vector` and `matrix`. This becomes a bit difficult for higher-dimensional arrays, so they are simply referred to as `3darray`, `4darray`,..., `7darray`.

```
PROCEDURE_SECTION
  P=Pcoff;
  dvar_vector ssum=colsum(P); // form a vector whose elements are the
                              // sums of the columns of P
  ff+=norm2(log(ssum)); // this is a penalty so that the hessian will
                        // not be singular and the coefficients of P
                        // will be well defined
  // normalize the transition matrix P so its columns sum to 1
  int j;
  for (j=0;j<=nstates-1;j++)
  {
    for (int i=0;i<=nstates-1;i++)
    {
      P(i,j)/=ssum(j);
    }
  }

  // get z into a useful format
  dvar_matrix ztrans(0,1,1,nperiods);
  ztrans(0)=y-a0;
  ztrans(1)=y-a0-a1;
  z=trans(ztrans);
  int t,i,k,l,m,n;

  qb1(0)=(1.0-P(1,1))/(2.0-P(0,0)-P(1,1)); // unconditional distribution
  qb1(1)=1.0-qb1(0);

  // for periods 2 through 4 there are no observations to condition
  // the state distributions on so we use the unconditional distributions
  // obtained by multiplying by the transition matrix P.
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) qb2(i,j)=P(i,j)*qb1(j);
  }

  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) qb3(i,j,k)=P(i,j)*qb2(j,k);
    }
  }
```

```
for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
      for (l=0;l<=1;l++) qb4(i,j,k,l)=P(i,j)*qb3(j,k,l);
    }
  }
}

// qb(5) is the probability of being in one of 32
// states (32=2x2x2x2x2) in periods 5,4,3,2,1 before observing
// y(5)
for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
      for (l=0;l<=1;l++) {
        for (m=0;m<=1;m++) qb(op1,i,j,k,l,m)=P(i,j)*qb4(j,k,l,m);
      }
    }
  }
}
// now calculate the realized values for epsilon for all
// possible combinations of states
for (t=op1;t<=nperiods;t++) {
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) {
          for (m=0;m<=1;m++) {
            eps(t,i,j,k,l,m)=z(t,i)-phi(z(t-1,j),
              z(t-2,k),z(t-3,l),z(t-4,m),f);
            eps2(t,i,j,k,l,m)=square(eps(t,i,j,k,l,m));
          }
        }
      }
    }
  }
}
// calculate the mean squared "residuals" for use in
// "undimensionalized" parameterization of sigma
dvariable eps2sum=sum(eps2);
var=smult*eps2sum/(32.0*(nperiods-4));
```

```
sigma=sqrt(var);

for (t=op1;t<=nperiods;t++) {
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++)
        prob(t,i,j,k)=exp(eps2(t,i,j,k)/(-2.*var))/sigma;
    }
  }
}

for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
      for (l=0;l<=1;l++) {
        for (m=0;m<=1;m++) qa(op1,i,j,k,l,m)= qb(op1,i,j,k,l,m)*
          prob(op1,i,j,k,l,m);
      }
    }
  }
}
ff1=0.0;
qbefore(op1,0)=sum(qb(op1,0));
qbefore(op1,1)=sum(qb(op1,1));
qafter(op1,0)=sum(qa(op1,0));
qafter(op1,1)=sum(qa(op1,1));
dvariable sumqa=sum(qafter(op1));
qa(op1)/=sumqa;
qafter(op1,0)/=sumqa;
qafter(op1,1)/=sumqa;
ff1-=log(1.e-50+sumqa);
for (t=op1+1;t<=nperiods;t++) { // notice that the t loop includes 2
  for (i=0;i<=1;i++) {   // i,j,k,l,m blocks
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) {
          for (m=0;m<=1;m++) {
            qb(t,i,j,k,l,m).initialize();
            // here is where having 6 dimensional arrays makes the
            // formula for moving the state distributions form period
            // t-1 to period t easy to program and understand.
            // Throw away n and accumulate its two values into next
```

```
            // time period after multiplying by transition matrix P
            for (n=0;n<=1;n++) qb(t,i,j,k,l,m)+=P(i,j)*qa(t-1,j,k,l,m,n);
          }
        }
      }
    }
  }
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) {
          for (m=0;m<=1;m++) qa(t,i,j,k,l,m)=qb(t,i,j,k,l,m)*
               prob(t,i,j,k,l,m);
        }
      }
    }
  }
  qbefore(t,0)=sum(qb(t,0));
  qbefore(t,1)=sum(qb(t,1));
  qafter(t,0)=sum(qa(t,0));
  qafter(t,1)=sum(qa(t,1));
  dvariable sumqa=sum(qafter(t));
  qa(t)/=sumqa;
  qafter(t,0)/=sumqa;
  qafter(t,1)/=sumqa;
  ff1-=log(1.e-50+sumqa); // add small constant to avoid log(0)
}
ff+=ff1; //ff1 is minus the log-likelihood
ff+=.1*norm2(f); // add small penalty to stabilize estimation
```

The PROCEDURE_SECTION is where the calculations of the objective function are carried out. First, the transition matrix P is calculated from the Pcoff. The function colsum forms a vector whose elements are the column sums of the matrix. This is used to normalize P so that its columns sum to 1. A penalty is added to the objective function for the column sums, so the Hessian matrix with respect to the independent variables will not be singular. This does not affect the "statistical" properties of the parameters of interest. The matrix z is calculated using a transformed matrix, because AD Model Builder deals with vector rows better than columns. The probability distribution for the states in period 1, qb1, is set equal to the unconditional distribution for a Markov process in terms of its transition matrix P, as discussed in [5]. The transition matrix is used to compute the probability distribution of the states in periods $(2,1)$, $(3,2,1)$, $(4,3,2,1)$, and finally, $(5,4,3,2,1)$. For the last quintuplet, this is the probability distribution before observing y(5). The quantities eps in the code correspond to the possible realized values of the random variable ϵ. The quantities qa and

qb correspond to q_a and q_b in the documentation. The sum function is defined for arrays of any dimension and simply forms the sum of all the components. In AD Model Builder, if xx is an n-dimensional array, then x(i) is an $(n-1)$-dimensional array. So, the statement

```
qbefore(t,0)=sum(qb(t,0));
```

takes the sum of the probabilities for the 16 quintuples of states, at time period t through t-4, for which the state at time period t is 0. These are used in the REPORT_SECTION, to write out a report of the estimated state probabilities at time period t, before and after observing y(t).

```
REPORT_SECTION
  dvar_matrix out(1,2,op1,nperiods);
  dvar_matrix out1(1,1,op1,nperiods);
  out(1)=trans(qbefore)(1);
  out(2)=trans(qafter)(1);
  {
    ofstream ofs("qbefore.rep");
    out1(1)=trans(qbefore)(0);
    ofs << trans(out1)<< endl;
  }
  {
    ofstream ofs("qafter.rep");
    out1(1)=trans(qafter)(0);
    ofs << trans(out1) << endl;
  }
  report << "#qbefore  qafter" << endl;
  report << setfixed << setprecision(3) << setw(7) << trans(out) << endl;
```

The REPORT_SECTION is used to report any result in a manner not already carried out by the model's default behavior. The probabilities of being in state 0 before and after observing y(t) are printed into the files qbefore.rep and qafter.rep. These vectors were stored in files, so they could be easily imported into graphing programs. The results are very similar to Figure 1 in [4], as one might hope.

```
RUNTIME_SECTION
  maximum_function_evaluations 20000
  convergence_criteria 1.e-6
```

The maximum_function_evaluations 20000 will simply let the program run a long time by setting the maximum number of function evaluations in the function minimizer equal to 20,000. (Nowhere near this many are actually needed.) The statement

```
  convergence_criteria 1.e-6
```

was needed, because the default value of 1.e-4 caused the program to exit from the minimization before convergence had been achieved.

```
TOP_OF_MAIN_SECTION
```

```
  arrmblsize=500000;
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(200000);
  gradient_structure::set_CMPDIF_BUFFER_SIZE(2100000);
```

The TOP_OF_MAIN_SECTION is for including code that will be included at the top of the main() function in the C++ program. Any desired legal code may be included. There are a number of common statements that are used to control aspects of AD Model Builder's performance. The statement

```
  arrmblsize=500000;
```

reserves 500,000 bytes of memory for variable objects. If it is not large enough, a message will be printed out at run time. See the index for references to more discussions of this matter. The statements

```
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(200000);
```

and

```
  gradient_structure::set_CMPDIF_BUFFER_SIZE(2100000);
```

set the amount of memory that AD Model Builder reserves for variable objects. Setting these is a matter of tuning for optimum performance. If you have a lot of memory available, making them larger may improve performance. However, models will run without including these statements, as long as there is enough memory for AD Model Builder's temporary files.

```
GLOBALS_SECTION
  #include <admodel.h>

  dvariable phi(const dvariable& a1,const dvariable& a2,const dvariable& a3,
    const dvariable& a4,const dvar_vector& f)
  {
    return  a1*f(1)+a2*f(2)+a3*f(3)+a4*f(4);
  }
```

The GLOBALS_SECTION is used to include statements at the top of the file containing the CPP program. This is generally where global declarations are made in C++, hence its name. However, it may be used for any legal statements, such as including header files for the user's data structures, etc. In this case, it has been used to define the function phi, which is used to simplify the code for the model's calculations. The header file admodel.hpp is included, to define the AUTODIF structures used in the definition of the function. This header is automatically included near the top of the file, but this would be too late, as GLOBALS_SECTION material is included first.

4.3 Results of the analysis

The parameter estimates for the initial parameters are written into a file `HAM4.PAR`. This is an ASCII file, which can be easily read. (The results are also stored in a binary file `HAM4.BAR`, which can be used to restart the model with more accurate parameters estimates.)

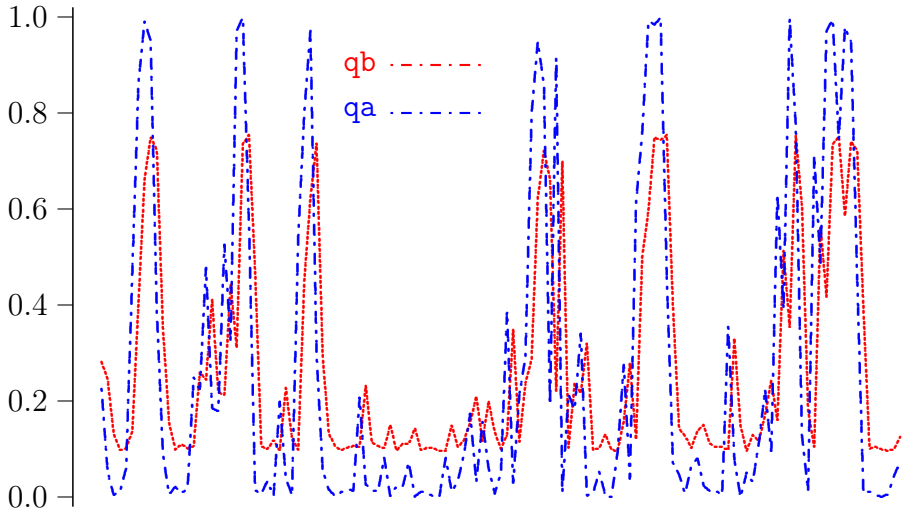
```
# Objective function value = 60.8934
# f:
 0.0139989 -0.0569580 -0.246292 -0.212250
# Pcoff:
 0.754133 0.0955834
 0.245118 0.900333
# a0:
-0.357964
# a1:
1.52138
# smult:
0.281342
```

The estimates are almost identical to those reported in [4][2] The first line reports the value of the log-likelihood function. This value can be used in hypothesis (likelihood-ratio) tests. The file `ham5.para` for the fifth-order autoregressive model fit to the data in [4] is shown below. There is one more parameter in this model. Twice the difference in the log-likelihood functions is $2(60.89 - 59.60) = 2.58$. For one extra parameter, the 95% significance level is 3.84, so the improvement in fit is not significant.

```
# Objective function value = 59.6039
# f:
 -0.0474771 -0.113829 -0.241966 -0.225535 -0.192585
# Pcoff:
 0.779245 0.0951739
 0.219775 0.900719
# a0:
-0.271318
# a1:
1.46301
# smult:
0.259541
```

The plot of `qa` and `qb` demonstrates the extra information about the probability distribution of the current state contained in in the current value of `y(t)`. (See Figure 4.1.)

[2] Our method for parameterizing the initial state probability distribution `qb1` is slightly different from Hamilton's, which would explain the small discrepancy.



The standard deviation and correlation report for the model are in the file `ham4.cor`, reproduced below:

index	name	value	std.dev	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	f	1.39e-02	1.20e-01	1.00														
2	f	-5.69e-02	1.37e-01	0.33	1.00													
3	f	-2.46e-01	1.06e-01	0.33	0.29	1.00												
4	f	-2.12e-01	1.10e-01	0.43	0.26	0.17	1.00											
5	Pcoff	7.54e-01	5.39e-01	0.00	0.04	0.01	0.00	1.00										
6	Pcoff	9.55e-02	7.58e-02	0.04	0.05	0.02	0.03	-0.04	1.00									
7	Pcoff	2.45e-01	1.97e-01	-0.01	-0.11	-0.03	-0.01	0.77	0.04	1.00								
8	Pcoff	9.00e-01	6.20e-01	-0.00	-0.00	-0.00	-0.00	0.00	0.83	-0.00	1.00							
9	a0	-3.57e-01	2.65e-01	0.27	0.56	0.25	0.21	0.08	0.07	-0.23	-0.00	1.00						
10	a1	1.52e+00	2.63e-01	-0.31	-0.57	-0.29	-0.25	-0.07	-0.04	0.21	0.00	-0.96	1.00					
11	smult	2.81e-01	1.25e-01	0.54	0.69	0.48	0.45	0.06	0.05	-0.17	-0.00	0.82	-0.84	1.00				
12	P	7.54e-01	9.65e-02	0.02	0.24	0.07	0.03	0.17	-0.08	-0.48	0.00	0.47	-0.44	0.36	1.00			
13	P	9.59e-02	3.77e-02	0.09	0.10	0.04	0.06	-0.02	0.49	0.08	-0.05	0.14	-0.09	0.11	-0.16	1.00		
14	P	2.45e-01	9.65e-02	-0.02	-0.24	-0.07	-0.03	-0.17	0.08	0.48	-0.00	-0.47	0.44	-0.36	-1.00	0.16	1.00	
15	P	9.04e-01	3.77e-02	-0.09	-0.10	-0.04	-0.06	0.02	-0.49	-0.08	0.05	-0.14	0.09	-0.11	0.16	-1.00	-0.16	1.00

Figure 4.1: Apriori and aposteriori probabilities of being in state 0 in period t.

4.4 Extending Hamilton's model to a fifth-order autoregressive process

Hamilton [4], page 372, remarks that investigating higher-order autoregressive processes might be a fruitful area of research. The first extension of the model is a fifth-order autoregressive process.

$$Y_t = a_0 + a_1 s_{ti} + Z_t \tag{4.8}$$

and the state variables Z_t satisfy the fourth-order autoregressive relationship

$$Z_t = f_1 Z_{t-1} + f_2 Z_{t-2} + f_3 Z_{t-3} + f_4 Z_{t-4} + f_5 Z_{t-5} + \epsilon_t \tag{4.9}$$

which extend equations (4.1) and (4.2). The TPL file `ham5.tpl` for the fifth-order autoregressive model is reproduced here. By employing higher-dimensional arrays, the conversion of the TPL file from a fourth-order autoregressive process to a fifth-order one is largely formal. An experienced AD Model Builder user can carry out the modifications in under one hour. Places where modifications were made are tagged with the comment `//!!5`.

```
DATA_SECTION
  init_number a1init // read in the initial value of a1 with the data
  init_int nperiods1 // the number of observations
  int nperiods // nperiods-1 after differencing
 !! nperiods=nperiods1-1;
  init_vector yraw(1,nperiods1) //read in the observations
  vector y(1,nperiods) // the differenced observations
 !! y=100.*(--log(yraw(2,nperiods1)) - log(yraw(1,nperiods)));
  int order
  int op1
 !! order=5; // !!5 order of the autoregressive process
 !! op1=order+1;
  int nstates // the number of states (expansion and contraction)
 !! nstates=2;
PARAMETER_SECTION
  init_vector f(1,order,1) // coefficients for the autoregressive
                           // process
  init_bounded_matrix Pcoff(0,nstates-1,0,nstates-1,.01,.99,2)
       // determines the transition matrix for the markov process
  init_number a0(5) // equation 4.3 in Hamilton (1989)
  init_bounded_number a1(0.0,10.0,4);
 !! if (a0==0.0) a1=a1init; // set initial value for a1 as specified
                    // in the top of the file nham4.dat
  init_bounded_number smult(0.01,1,3) // used in computing sigma
  matrix z(1,nperiods,0,1) // computed via equation 4.3 in
                           // Hamilton (1989)
```

```
  matrix qbefore(op1,nperiods,0,1); // prob. of being in state before
  matrix qafter(op1,nperiods,0,1); // and after observing y(t)
  number sigma // variance of epsilon(t) in equation 4.3
  number var // square of sigma
  sdreport_matrix P(0,nstates-1,0,nstates-1);
  number ff1;
  vector qb1(0,1);
  matrix qb2(0,1,0,1);
  3darray qb3(0,1,0,1,0,1);
  4darray qb4(0,1,0,1,0,1,0,1);
  5darray qb5(0,1,0,1,0,1,0,1,0,1); // !!5
  7darray qb(op1,nperiods,0,1,0,1,0,1,0,1,0,1,0,1);
  7darray qa(op1,nperiods,0,1,0,1,0,1,0,1,0,1,0,1);
  7darray eps(op1,nperiods,0,1,0,1,0,1,0,1,0,1,0,1);
  7darray eps2(op1,nperiods,0,1,0,1,0,1,0,1,0,1,0,1);
  7darray prob(op1,nperiods,0,1,0,1,0,1,0,1,0,1,0,1);
  objective_function_value ff;
PROCEDURE_SECTION
  P=Pcoff;
  dvar_vector ssum=colsum(P); // form a vector whose elements are the
                              // sums of the columns of P
  ff+=norm2(log(ssum)); // this is a penalty so that the Hessian will
                        // not be singular and the coefficients of P
                        // will be well defined
  // normalize the transition matrix P so its columns sum to 1
  int j;
  for (j=0;j<=nstates-1;j++)
  {
    for (int i=0;i<=nstates-1;i++)
    {
      P(i,j)/=ssum(j);
    }
  }

  dvar_matrix ztrans(0,1,1,nperiods);
  ztrans(0)=y-a0;
  ztrans(1)=y-a0-a1;
  z=trans(ztrans);
  int t,i,k,l,m,n,p;

  qb1(0)=(1.0-P(1,1))/(2.0-P(0,0)-P(1,1)); // unconditional distribution
  qb1(1)=1.0-qb1(0);
```

```
// for periods 2 through 4 there are no observations to condition
// the state distributions on so we use the unconditional distributions
// obtained by multiplying by the transition matrix P.
for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) qb2(i,j)=P(i,j)*qb1(j);
}

for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) qb3(i,j,k)=P(i,j)*qb2(j,k);
  }
}

for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
      for (l=0;l<=1;l++) qb4(i,j,k,l)=P(i,j)*qb3(j,k,l);
    }
  }
}
// !!5
for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
      for (l=0;l<=1;l++) {
        for (m=0;m<=1;m++) qb5(i,j,k,l,m)=P(i,j)*qb4(j,k,l,m);
      }
    }
  }
}
// qb(6) is the probability of being in one of 64
// states (64=2x2x2x2x2x2) in periods 5,4,3,2,1 before observing
// y(6)
for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
      for (l=0;l<=1;l++) {
        for (m=0;m<=1;m++) { // !!5
          for (n=0;n<=1;n++) qb(op1,i,j,k,l,m,n)=P(i,j)*qb5(j,k,l,m,n);
        }
      }
```

```
    }
  }
}
// now calculate the realized values for epsilon for all
// possible combinations of states
for (t=op1;t<=nperiods;t++) {
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) {
          for (m=0;m<=1;m++) {
            for (n=0;n<=1;n++) { // !!5
              eps(t,i,j,k,l,m,n)=z(t,i)-phi(z(t-1,j),
                z(t-2,k),z(t-3,l),z(t-4,m),z(t-5,n),f);
              eps2(t,i,j,k,l,m,n)=square(eps(t,i,j,k,l,m,n));
            }
          }
        }
      }
    }
  }
}
// calculate the mean squared "residuals" for use in
// "undimensionalized" parameterization of sigma
dvariable eps2sum=sum(eps2);
var=smult*eps2sum/(64.0*(nperiods-4)); //!!5
sigma=sqrt(var);

for (t=op1;t<=nperiods;t++) {
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) //!!5
          prob(t,i,j,k,l)=exp(eps2(t,i,j,k,l)/(-2.*var))/sigma;
      }
    }
  }
}

for (i=0;i<=1;i++) {
  for (j=0;j<=1;j++) {
    for (k=0;k<=1;k++) {
```

```
      for (l=0;l<=1;l++) {
        for (m=0;m<=1;m++) {
          for (n=0;n<=1;n++) qa(op1,i,j,k,l,m,n)= qb(op1,i,j,k,l,m,n)*
            prob(op1,i,j,k,l,m,n);
        }
      }
    }
  }
}
ff1=0.0;
qbefore(op1,0)=sum(qb(op1,0));
qbefore(op1,1)=sum(qb(op1,1));
qafter(op1,0)=sum(qa(op1,0));
qafter(op1,1)=sum(qa(op1,1));
dvariable sumqa=sum(qafter(op1));
qa(op1)/=sumqa;
qafter(op1,0)/=sumqa;
qafter(op1,1)/=sumqa;
ff1-=log(1.e-50+sumqa);
for (t=op1+1;t<=nperiods;t++) { // notice that the t loop includes 2
  for (i=0;i<=1;i++) {   // i,j,k,l,m blocks
    for (j=0;j<=1;j++) {
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) {
          for (m=0;m<=1;m++) {
            for (n=0;n<=1;n++) { //!!5
              qb(t,i,j,k,l,m,n).initialize();
              // here is where having 6 dimensional arrays makes the
              // formula for moving the state distributions form period
              // t-1 to period t easy to program and understand.
              // Throw away n and accumulate its two values into next
              // time period after multiplying by transition matrix P
              for (p=0;p<=1;p++) qb(t,i,j,k,l,m,n)+=P(i,j)*
                qa(t-1,j,k,l,m,n,p);
            }
          }
        }
      }
    }
  }
  for (i=0;i<=1;i++) {
    for (j=0;j<=1;j++) {
```

```
      for (k=0;k<=1;k++) {
        for (l=0;l<=1;l++) {
          for (m=0;m<=1;m++) { // !!5
            for (n=0;n<=1;n++) qa(t,i,j,k,l,m,n)=qb(t,i,j,k,l,m,n)*
                prob(t,i,j,k,l,m,n);
          }
        }
      }
    }
    qbefore(t,0)=sum(qb(t,0));
    qbefore(t,1)=sum(qb(t,1));
    qafter(t,0)=sum(qa(t,0));
    qafter(t,1)=sum(qa(t,1));
    dvariable sumqa=sum(qafter(t));
    qa(t)/=sumqa;
    qafter(t,0)/=sumqa;
    qafter(t,1)/=sumqa;
    ff1-=log(1.e-50+sumqa);
  }
  ff+=ff1;
  ff+=.1*norm2(f);
REPORT_SECTION
  dvar_matrix out(1,2,op1,nperiods);
  out(1)=trans(qbefore)(1);
  out(2)=trans(qafter)(1);
  {
    ofstream ofs("qbefore4.tex");
    for (int t=5;t<=nperiods;t++)
    {
      ofs << (t-4)/100. << " " << qbefore(t,0) << endl;
    }
  }
  {
    ofstream ofs("qafter4.tex");
    for (int t=5;t<=nperiods;t++)
    {
      ofs << (t-4)/100. << " " << qafter(t,0) << endl;
    }
  }
  report << "#qbefore  qafter" << endl;
  report << setfixed << setprecision(3) << setw(7) << trans(out) << endl;
```

```
RUNTIME_SECTION
  maximum_function_evaluations 20000
  convergence_criteria 1.e-6
TOP_OF_MAIN_SECTION
  arrmblsize=500000;
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(400000);
  gradient_structure::set_CMPDIF_BUFFER_SIZE(2100000);
  gradient_structure::set_MAX_NVAR_OFFSET(500);
GLOBALS_SECTION
  #include <fvar.hpp>
   // !!5
  dvariable phi(const dvariable& a1,const dvariable& a2,const dvariable& a3,
    const dvariable& a4,const dvariable& a5,const dvar_vector& f)
  {
    return  a1*f(1)+a2*f(2)+a3*f(3)+a4*f(4)+a5*f(5);
  }
```

Chapter 5

Econometric Models: Simultaneous Equations

5.1 Simultaneous equations models

For each t, $1 \leq t \leq T$ let y_t be an n-dimensional vector and x_t be an n-dimensional vector. Let B and Γ be $(n \times n)$ and $(n \times m)$ matrices, and suppose that the relationship

$$By_t + \Gamma x_t = u_t$$

holds, where the u_t are n-dimensional random vectors of disturbances. The y_t are the endogenous variables in the system. The x_t are predetermined variables in the sense that they are independent of u_t. Note that for autoregressive models, the x_t may contain values of y_j for $j < i$. In general, not all of the coefficients of B and Γ are estimable. Interesting cases have special structure that are determined by the particular parameterization of of B, Γ, and D. In particular, it is generally assumed that $B_{ii} = 1$ for $1 \leq i \leq n$ and that B^{-1} exists.

5.2 Full information maximum likelihood (FIML)

Assume that for each t, u_t has a multivariate normal distribution with mean 0 and covariance matrix D. The log-likelihood function for B, Γ, and D is given by

$$L(B, \Gamma, D) = T/2 \log\left(|B|^2\right) - T/2 \log\left(|D|\right) - 1/2 \sum_{t=1}^{T} [By_t + \Gamma x_t]' D^{-1} [By_t + \Gamma x_t] \quad (5.1)$$

5.3 Concentrating out D for the FIML

If there are no constraints on D, the value of D that maximizes (5.1) can be solved for in terms of the other parameters and observations. This value, $\hat{D}$, is given by

$$\hat{D} = 1/T \sum_{t=1}^{T} [By_t + \Gamma x_t]'[By_t + \Gamma x_t] \tag{5.2}$$

By substituting this value into equation (5.1), it can be shown that

$$1/2 \sum_{t=1}^{T} [By_t + \Gamma x_t]' \hat{D}^{-1} [By_t + \Gamma x_t]$$

is a constant that can be ignored for the maximization, so equation (5.2), this:

$$\tilde{L}(B, \Gamma) = T/2 \log\left(|B|^2\right) - T/2 \log\left(|\hat{D}|\right) \tag{5.3}$$

plus the FIML estimates for B and Γ can be found by maximizing $\tilde{L}(B, \Gamma)$.

When there are constraints on the parameters of D, then $\tilde{D}$ is no longer the maximum likelihood estimate for D. So, it is necessary to maximize equation (5.1), which is, in general, a numerically unstable problem. To successfully carry out the optimization, it is necessary to obtain reasonable initial estimates for the parameters of B and Γ, and to use a good method for parameterizing D. Initial estimates for B and Γ can be obtained from ordinary least squares (OLS), that is, finding the values of B and Γ that minimize

$$\sum_{t=1}^{T} \|y_t - B^{-1}\Gamma x_t\|^2$$

To parameterize D, note that $\hat{D}$ is an estimate of D, so we can parameterize D by

$$D = A\hat{D}A'$$

where A is a lower triangular matrix. If U is the Choleski decomposition of D and $\hat{U}$ is the Choleski decomposition of $\hat{D}$, then $A = \hat{U}^{-1}U$. It follows that A should be close to the identity matrix, which is a good initial estimate for A.

5.4 Evaluating the model's performance

To evaluate the model's performance, simulated data were generated. The form of the model is

$$\begin{aligned}
y_{t1} + y_{t4} + y_{t5} - 2 + 0.45y_{t-1,1} &= u_{t1} \\
0.1y_{t1} + y_{t2} + 2.0y_{t5} - 1 - 0.6y_{t-1,1} + 0.25y_{t-1,2} &= u_{t2} \\
0.3y_{t1} - 0.2y_{t2} + y_{t3} + 1 &= u_{t3} \\
1.4y_{t2} - 3.1y_{t3} + y_{t4} + 1 &= u_{t4} \\
y_{t3} + y_{t4} + y_{t5} &= u_{t5}
\end{aligned} \tag{5.4}$$

with a covariance matrix

$$D = \begin{pmatrix} 0.512 & 0.32 & 0.256 & -1.28 & 0 \\ 0.32 & 0.328 & -0.16 & -0.8 & 0 \\ 0.256 & -0.16 & 1.728 & 0.16 & 0.8 \\ -1.28 & -0.8 & 0.16 & 4.8 & 0.8 \\ 0 & 0 & 0.8 & 0.8 & 0.928 \end{pmatrix}$$

$$B = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ 0.1 & 1 & 0 & 0 & 2 \\ 0.3 & -0.2 & 1 & 0 & 0 \\ 0 & 1.4 & -3.1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{pmatrix}$$

$$\Gamma = \begin{pmatrix} -2 & 0.45 & 0 \\ -1 & -0.6 & 0.25 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

For this model, $n = 5$, $m = 3$, and $x_t = (1, y_{t-1,1}, y_{t-1,2})$.

The eigenvalues of D are (0.006610.135830.49622.211625.44573). Having a small eigenvalue tends to produce simulated data that are difficult to analyze.

Forty time periods of data were generated by the simulator. The simulated y values are:

```
1.63252 3.00223 1.70246 1.34813 -1.12202
-2.87857 -7.72402 -3.88482 -1.24196 4.71024
1.12975 -7.92719 -3.85188 -2.33007 4.2984
1.48112 -2.25692 -1.15585 -2.26166 3.01061
-2.91887 -5.65015 -2.74198 -0.695815 4.51346
2.29715 0.524946 0.0268777 1.07624 -0.0898846
1.32854 6.17993 2.51613 1.67248 -2.39914
0.5661 -2.53219 -0.966376 0.00820516 1.76543
0.353591 -3.81146 -2.04431 -1.48574 2.67208
-2.22887 -2.33436 -1.66284 0.646399 2.26448
2.29896 -6.42238 -2.41106 -1.70633 3.50028
0.145878 1.85161 0.646578 -0.380955 0.709761
-0.779376 -7.60611 -3.79636 -1.63017 4.02658
-0.107371 -5.61361 -2.35816 -1.77719 3.67762
0.662221 -5.78832 -2.19632 -2.03071 4.37961
-0.570661 -7.42505 -3.28544 -2.94125 5.19422
0.0953742 -1.80617 -1.06915 -0.0320784 2.00018
```

```
-0.406986 -4.96143 -2.8084 -0.948902 3.1811
1.07219 -7.92608 -2.95484 -3.17022 5.12702
-0.495144 1.33611 -0.357291 -0.0260083 0.360653
-0.637878 -8.76117 -3.81638 -1.77116 4.82796
1.59717 -3.18571 -1.72708 -1.93975 2.79462
-1.13013 -2.20942 -1.30198 -0.603895 2.29486
-1.0103 -7.90106 -3.65303 -1.07367 4.66283
-1.02985 -3.00268 -1.63388 0.309992 2.97876
0.176882 -7.96282 -3.60299 -1.86289 4.86943
1.16904 -1.07952 -0.0969977 -0.74563 2.38399
-0.636119 -2.84841 -1.43676 -0.38474 2.51142
-1.72929 -5.39866 -2.51289 0.0978131 3.786
3.56302 3.79343 2.05613 1.43836 -1.2029
0.15806 -0.863882 -0.302119 -1.19212 1.38518
1.37323 -1.94413 -0.537631 -0.751294 1.42083
-0.404075 -8.53817 -3.58618 -3.33976 5.69071
0.362091 -5.78568 -2.46635 -2.33359 4.21899
-2.26158 -12.7075 -6.07426 -3.62455 8.49292
1.20438 -5.44629 -2.30249 -2.02905 3.82742
1.41463 -1.71734 -0.788698 -1.90306 2.2595
0.897156 1.28039 0.693579 0.318737 0.385857
-0.0330384 -1.55642 -0.189474 0.312385 1.57168
1.5747 0.827181 1.26032 0.813312 0.270432
```

For the x values, the first time periods data $x_0 = (1, 1, 2)$ were supplied. The simulated x values are:

```
1 1 2
1 1.63252 3.00223
1 -2.87857 -7.72402
1 1.12975 -7.92719
1 1.48112 -2.25692
1 -2.91887 -5.65015
1 2.29715 0.524946
1 1.32854 6.17993
1 0.5661 -2.53219
1 0.353591 -3.81146
1 -2.22887 -2.33436
1 2.29896 -6.42238
1 0.145878 1.85161
1 -0.779376 -7.60611
1 -0.107371 -5.61361
1 0.662221 -5.78832
1 -0.570661 -7.42505
```

```
1 0.0953742 -1.80617
1 -0.406986 -4.96143
1 1.07219 -7.92608
1 -0.495144 1.33611
1 -0.637878 -8.76117
1 1.59717 -3.18571
1 -1.13013 -2.20942
1 -1.0103 -7.90106
1 -1.02985 -3.00268
1 0.176882 -7.96282
1 1.16904 -1.07952
1 -0.636119 -2.84841
1 -1.72929 -5.39866
1 3.56302 3.79343
1 0.15806 -0.863882
1 1.37323 -1.94413
1 -0.404075 -8.53817
1 0.362091 -5.78568
1 -2.26158 -12.7075
1 1.20438 -5.44629
1 1.41463 -1.71734
1 0.897156 1.28039
1 -0.0330384 -1.55642
```

5.5 Results of (FIML) for unconstrained D

For the estimation process, all the elements of the matrices B and Γ with value 0 were fixed at their correct value. The FIML estimates for unconstrained covariance matrix D are given below.

$$B = \begin{pmatrix} 1 & 0 & 0 & 0.364395 & 0.364395 \\ 0.238411 & 1 & 0 & 0 & 1.37593 \\ 0.042875 & -0.330484 & 1 & 0 & 0 \\ 0 & 1.93026 & -4.90367 & 1 & 0 \\ 0 & 0 & 1.06339 & 1.09851 & 1 \end{pmatrix}$$

$$\Gamma = \begin{pmatrix} -0.917978 & 0.431377 & 0 \\ 0.473915 & -0.491422 & 0.19981 \\ 0.441089 & 0 & 0 \\ -0.126701 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$D = \begin{pmatrix} 0.938236 & 0.843743 & 0.506127 & -1.38383 & 0.314262 \\ 0.843743 & 1.55844 & 0.732235 & -0.591771 & 1.37195 \\ 0.506127 & 0.732235 & 0.430091 & -0.805866 & 0.62244 \\ -1.38383 & -0.591771 & -0.805866 & 4.18591 & -0.0363513 \\ 0.314262 & 1.37195 & 0.62244 & -0.0363513 & 1.75939 \end{pmatrix}$$

5.6 Results of (FIML) for constrained D

Since $D_{51} = 0$ and $D_{52} = 0$, these values were not well estimated by the unconstrained FIML procedure. Suppose that we know that their values should be 0 and that the value of $D_{55} \leq 1.0$. We incorporate this knowledge into the model by using penalty functions.

$$B = \begin{pmatrix} 1 & 0 & 0 & 0.594218 & 0.594218 \\ -0.321482 & 1 & 0 & 0 & 1.97809 \\ 0.0416175 & -0.365572 & 1 & 0 & 0 \\ 0 & 2.48468 & -6.10763 & 1 & 0 \\ 0 & 0 & 0.968057 & 1.02738 & 1 \end{pmatrix}$$

$$\Gamma = \begin{pmatrix} -1.3418 & 0.448342 & 0 \\ -1.14717 & -0.593754 & 0.183788 \\ 0.372114 & 0 & 0 \\ -0.0640792 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$D = \begin{pmatrix} 0.593424 & -0.325467 & 0.298836 & -1.43231 & 0.00401209 \\ -0.325467 & 0.650371 & -0.234747 & 0.441841 & 4.48456 \times 10^{-06} \\ 0.298836 & -0.234747 & 0.258147 & -0.900105 & 0.255262 \\ -1.43231 & 0.441841 & -0.900105 & 6.13619 & 0.180376 \\ 0.00401209 & 4.48456 \times 10^{-06} & 0.255262 & 0.180376 & 1.00262 \end{pmatrix}$$

5.7 Code for (FIML) for constrained D

This is the code in the TPL file, split up by sections and commented on. The `DATA_SECTION` defines the data and some size aspects of the model structure. Objects that are prefixed by `init_` will be read in from the data file.

```
// This version incorporates constraints via penalty functions.
//This is sample code to determine the parameters of a
// simultaneous equations model. The notation follows
// that of Hamilton, Times Series Analysis, chapter 9.
```

```
// the general form of the model is
//
//    By_t + Gamma x_t =u_t
//
//for t=1,...,T. The u_t have covariance matrix D.

DATA_SECTION
  init_int T // the number of observations
  init_int dimy // dimension of the vector of
                // endogenous variables
  init_int dimx // dimension of the vector of
                // predetermined variables
  init_int num_Bpar // the number of parameters in
                // the elements of B to be estimated
  init_int num_Gpar // the number of parameters in
                // the elements of Gamma to be estimated
  init_matrix y(1,T,1,dimy) // the y_t
  init_matrix x(1,T,1,dimx) // the x_t
  int dimy1
 !! dimy1=dimy*(dimy+1)/2; // size of symmetric matrix
```

The PARAMETER_SECTION describes the model's parameters. Objects which are prefixed by init_ are the independent variables of the model. For example, Bpar is used to parameterize the nonzero elements of B. ch_Dpar is used to parameterize the lower triangular matrix of the correction from emp_D to the covariance matrix D. The minimization is done in a number of phases. The parameter kx is used to have a parameter that becomes active in phase 4, so that the minimization will take place in four stages. This parameter does not enter into the "real" part of the model.

```
PARAMETER_SECTION
  init_vector Bpar(1,num_Bpar)
  init_vector Gpar(1,num_Gpar)
  init_vector ch_Dpar(1,dimy1,2)
  matrix B(1,dimy,1,dimy)
  matrix D(1,dimy,1,dimy) // the covariance matrix for the
                          // disturbances u_t
  matrix emp_D(1,dimy,1,dimy) // the covariance matrix for the
  matrix Gamma(1,dimy,1,dimx)
  matrix ch_D(1,dimy,1,dimy)
  matrix z(1,T,1,dimy);
  objective_function_value f
  init_number kx(4);
```

The PROCEDURE_SECTION is where the model's calculations are carried out. It is split up into a set of functions where the model-specific pieces of code (different code for different models) are located. Finally, the optimization for parameter estimation is calculated. This depends on the phase of the optimization procedure. A `switch` statement is used to vary the form of the objective function depending on the phase. The function `current_phase()` returns the number of the current phase of the optimization. The function `last_phase()` returns 1 ("true") if the current phase is the last phase of the optimization. Quadratic penalty functions are put on the model's parameters, and these penalty weights are decreased in subsequent phases. This procedure helps to stabilize the optimization when several model parameters are highly correlated.

```
PROCEDURE_SECTION
  fill_B();   // this will vary from model to model
  fill_Gamma(); // this will vary from model to model

  calculate_empirical_copvariance_matrix();

  fill_D(); // this will vary from model to model

  calculate_constraints(); // this will vary from model to model

  int sgn;
  switch (current_phase())
  {
  case 1:
    {
      f+=0.1*norm2(Bpar);
      f+=0.1*norm2(Gpar);
      f+=0.1*norm2(ch_Dpar);
      dvar_matrix Binv=inv(B);
      for (int t=1;t<=T;t++)
      {
        dvar_vector z=y(t)+Binv*Gamma*x(t);
        f+=z*z;
      }
      break;
    }
  default:
    {
      f+= -0.5*T*log(square(det(B)))
       +0.5*T*ln_det(D,sgn);

      dvar_matrix Dinv=inv(D);
```

```
      dvariable f1=0.0;
      for (int t=1;t<=T;t++)
      {
        dvar_vector z=B*y(t)+Gamma*x(t);
        f1+=z*(Dinv*z);
      }
      f+=0.5*f1;
      if (!last_phase())
      {
        f+=0.1*norm2(Bpar);
        f+=0.1*norm2(Gpar);
        f+=0.1*norm2(ch_Dpar);
      }
      else
      {
        f+=0.001*norm2(Bpar);
        f+=0.001*norm2(Gpar);
        f+=0.001*norm2(ch_Dpar);
      }
    }
  }

  f+=square(kx);

FUNCTION fill_B
  B.initialize();
  for (int i=1;i<=dimy;i++)
    B(i,i)=1.0;

  // this is part of the special structure of the model
  int ii=1;
  B(2,1)=Bpar(1);
  B(3,1)=Bpar(2);

  B(3,2)=Bpar(3);
  B(4,2)=Bpar(4);

  B(4,3)=Bpar(5);
  B(5,3)=Bpar(6);

  B(5,4)=Bpar(7);
  B(1,4)=Bpar(8);
```

```
  B(1,5)=Bpar(8);
  B(2,5)=Bpar(9);


FUNCTION fill_Gamma
  Gamma.initialize();

  // this is the part of special structure of the model
  Gamma(1,1)=Gpar(1);
  Gamma(2,1)=Gpar(2);
  Gamma(3,1)=Gpar(3);
  Gamma(4,1)=Gpar(4);

  Gamma(1,2)=Gpar(5);
  Gamma(2,2)=Gpar(6);


  Gamma(2,3)=Gpar(7);


FUNCTION fill_D

  ch_D.initialize();
  // this is the special structure of the model
  int ii=1;
  for (int i=1;i<=dimy;i++)
  {
    for (int j=1;j<=i;j++)
      ch_D(i,j)=ch_Dpar(ii++);
    ch_D(i,i)+=1;
  }

  D=ch_D*emp_D*trans(ch_D); // so Ch_D is the Choleski
                    // decomposition of D
FUNCTION calculate_empirical_covariance_matrix

  for (int t=1;t<=T;t++)
    z(t)=B*y(t)+Gamma*x(t);

  emp_D=empirical_covariance(z);
```

```
FUNCTION calculate_constraints

  double wt=1.0;
  switch (current_phase())
  {
  case 1:
    wt=1.0;
    break;
  case 2:
    wt=10.0;
    break;
  case 3:
    wt=100.0;
    break;
  default:
    wt=1000.0;
    break;
  }
  if (D(5,5)>1.0)
    f+=wt*square(D(5,5)-1.00);

  f+=wt*square(D(5,1));
  f+=wt*square(D(5,2));
```

The REPORT_SECTION prints out a report of the model's results.

```
REPORT_SECTION
  report << "B" << endl;
  report << B << endl;
  report << "Gamma" << endl;
  report << Gamma << endl;
  report << "D" << endl;
  report << D << endl;
  report << "eigenvalues of D" << endl;
  report << eigenvalues(D) << endl;
  report << "y" << endl;
  report << y << endl;
  report << "x" << endl;
  report << x << endl;
```

Chapter 6

Truncated Regression

6.1 Truncated linear regression

The linear regression model we consider here has the form

$$Y_i = \sum_{j=1}^{m} a_j x_{ij} + \epsilon_i$$

where the Y_i for $i = 1, \ldots, n$ are the n observations and the a_j are m parameters to be estimated. The ϵ_i are assumed to be normally distributed random variables with mean 0 and variance v.

Let $r_i = Y_i - \sum_{j=1}^{m} a_j x_{ij}$. The log-likelihood function for the standard regression model is given by

$$-.5n \log(v) - \sum_{i=1}^{n} \frac{r_i^2}{2v}$$

Now assume that we only consider the Y_i for $Y_i \geq 0$, i.e., the left truncated situation. The probability that $Y_i \geq 0$ is equal to the probability that $\epsilon_I > -\sum_{j=1}^{m} a_j x_{ij}$. This is equal to $1 - \Phi(-\sum_{j=1}^{m} a_j x_{ij}/v)$, where

$$\Phi(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{u} \exp\left(-t^2/2\right) \, \mathrm{d}t$$

For this truncated regression, the log-likelihood function has the logarithm of this quantity subtracted from it, so it becomes

$$-.5n \log(v) - \sum_{i=1}^{n} \frac{r_i^2}{2v} - \log\left(1 - \Phi\Big(-\sum_{j=1}^{m} a_j x_{ij}/v\Big)\right)$$

If instead we consider the right truncated case, where only the $Y_i < 0$ are considered, the log-likelihood function becomes

$$-.5n \log(v) - \sum_{i=1}^{n} \frac{r_i^2}{2v} - \log\left(\Phi\Big(-\sum_{j=1}^{m} a_j x_{ij}/v\Big)\right)$$

To parameterize v, we introduce a new parameter a satisfying the condition $v = a\hat{v}$, where $\hat{v} = \frac{1}{n}\sum_{i=1}^{n} r_i^2$ is the usual maximum likelihood estimate for v. This leads to more numerically stable behavior. In terms of a, the expression for the log-likelihood simplifies to

$$-.5n\log(a) - .5n\log(\hat{v}) - \frac{n}{2a} - \log\left(1 - \Phi\left(-\sum_{j=1}^{m} a_j x_{ij}/(a\hat{v})\right)\right)$$

6.2 The AD Model Builder truncated regression program

Here are the contents of the file `truncreg.tpl`:

```
DATA_SECTION
  init_int nobs
  init_int m
  init_int trunc_flag
  init_matrix data(1,nobs,1,m+1)
  vector Y(1,nobs)
  matrix X(1,nobs,1,m)
 LOC_CALCS
  Y=column(data,1);
  for (int i=1;i<=nobs;i++)
  {
    X(i)=data(i)(2,m+1).shift(1);
  }
PARAMETER_SECTION
  sdreport_number sigma
  number vhat
  init_bounded_number log_a(-5.0,5.0);
  sdreport_number a
  init_vector u(1,m)
  objective_function_value f
PROCEDURE_SECTION
  a=exp(log_a);
  dvar_vector pred=X*u;
  dvar_vector res=Y-pred;
  dvariable r2=norm2(res);
  vhat=r2/nobs;
  dvariable v=a*vhat;
  sigma=sqrt(v);

  dvar_vector spred=pred/sigma;
```

```
  f=0.0;
  switch (trunc_flag)
  {
  case -1: // left_truncated
    {
      for (int i=1;i<=nobs;i++)
      {
        f+=log(1.00001-cumd_norm(-spred(i)));
      }
    }
    break;
  case 1:  // right truncated
    {
      for (int i=1;i<=nobs;i++)
      {
        f+=log(0.99999*cumd_norm(-spred(i)));
      }
    }
    break;
  case 0:  // no truncation
    break;
  default:
    cerr << "Illegal value for truncation flag" << endl;
    ad_exit(1);
  }
  f+=0.5*nobs*log(v)+0.5*r2/v;


REPORT_SECTION
  report << "#u " << endl << u << endl;
  report << "#sigma " << endl << sigma << endl;
  report << "#a " << endl << a << endl;
  report << "#vhat " << endl << vhat << endl;
  report << "#shat " << endl << sqrt(vhat) << endl;
```

Chapter 7

Multivariate GARCH

The Vector Autoregressive Moving Average Garch process combines the Vector Autoregressive Moving Average (VARMA) processes with the Vector Garch (generalized autoregressive conditional heteroscedastic) processes.

7.1 Formulation of the VARMA GARCH process

The VARMA GARCH process of type (p, q, r, s) is given by a series Y_t for $t = -p+1, \ldots, n$, where for each value of t, Y_t is an m-dimensional vector. For $t > 0$, the Y_t are assumed to satisfy a relationship of the form

$$Y_t = \mu + \sum_{l=1}^{p} A_l(Y_{t-l} - \mu) + \sum_{l=0}^{q} B_l \epsilon_{t-l} \tag{7.1}$$

where the μ is an m-dimensional vector, A_l and B_l are $m \times m$ matrices, B_0 is the identity matrix, and the ϵ_t are multivariate (normal) random vectors, with means 0. Covariance matrices Σ_t and $\mathrm{E}(\epsilon_t \epsilon_{t'}) = 0$ if $t \neq t'$. Let

$$r_t = Y_t - \mu - \sum_{l=1}^{p} A_l(Y_{t-l} - \mu) \tag{7.2}$$

be the vector of model residuals or "shocks."[1] These residuals are assumed to contribute to the covariance matrix in the next time period. The Σ_t evolve according to one of several relationships.

The DVEC relationship

$$\Sigma_t = \Omega + \sum_{l=1}^{r} F_l \bigotimes r_{t-l} r'_{t-l} + \sum_{l=1}^{s} G_l \bigotimes \Sigma_{t-l} \tag{7.3}$$

[1] For the moving average model ($q > 0$), one might argue that since the previous values of r_t have been observed, the shock part of r_t, say, d_t, is given by $d_t = r_t - \sum_{l=1}^{q} B_l r_{t-l}$, but this has not been done at present.

In equation (7.3), the matrices F_l and G_l are symmetric and the operator '$\bigotimes$' denotes the element-wise product of matrices. This parameterization does not restrict the resulting matrix to be positive definite, so some care is necessary to ensure the stability of the resulting model.

The BEKK relationship

$$\Sigma_t = \Omega + \sum_{l=1}^{r} F_l \, r_{t-l} \, r'_{t-l} \, F'_l + \sum_{l=1}^{s} G_l \, \Sigma_{t-l} \, G'_l \tag{7.4}$$

DVECI and BEKKAI parameterizations

The basic DVEC and BEKK parameterizations can be extended by modifying components of the r_t to reflect the asymmetric response to positive and negative values.

$$\begin{aligned} \eta_{ij} &= \epsilon_{ij}/\alpha_j && \text{if } \epsilon_{ij} \geq 0 \\ \eta_{ij} &= \epsilon_{ij}\alpha_j && \text{if } \epsilon_{ij} < 0 \end{aligned} \tag{7.5}$$

This modified form will be referred to as the DVECI and BEKKAI parameterizations.

$$\Sigma_t = \Omega + \sum_{l=1}^{r} F_t \bigotimes \eta_{t-l} \, \eta'_{t-l} + \sum_{l=1}^{s} G_l \bigotimes \Sigma_{t-l} \tag{7.6}$$

$$\Sigma_t = \Omega + \sum_{l=1}^{r} F_l \, \eta_{t-l} \, \eta'_{t-l} \, F'_l + \sum_{l=1}^{s} G_l \, \Sigma_{t-l} \, G'_l \tag{7.7}$$

7.2 Setting a value for Σ_1

The value for the parameters in Σ_1 are often poorly determined and simply letting them be free parameters can lead to instability and initial transient effects in the model. To stabilize the parameterization, we have calculated Σ_1 through $\Sigma_{\max\{r,s\}}$ from the condition

$$\widehat{\Omega} = \Sigma + \sum_{l=1}^{q} B_l \Sigma B'_l \tag{7.8}$$

where

$$\widehat{\Omega} = \frac{1}{n} \sum_{t=1}^{n} \hat{\epsilon}_t \, \hat{\epsilon}'_t \tag{7.9}$$

denotes the empirical covariance matrix formed from the models residuals

$$\hat{\epsilon}_t = Y_t - \mu - \sum_{l=1}^{p} A_l (Y_{t-l} - \mu). \tag{7.10}$$

7.3 Ensuring that the Σ_t are positive definite

The DVEC parameterization can produce matrices that are not positive definite, and the BEKK parameterization can produce matrices that are almost not positive definite (much as a positive number can get arbitrarily close to zero). At worst, this will lead to a failure in the model to converge and at best, it makes the estimation somewhat unstable. To improve model performance, the BEKK and DVEC operations are followed by a modification of the resulting Σ_t that makes them more positive definite. The first problem is to get a notion of what is meant by "small" for a particular problem. This is accomplished by first scaling the Σ_t to produce a matrix Λ_t where

$$\Lambda_{ij} = \frac{\Sigma_{t_{ij}}}{\sqrt{\Sigma_{t_{ij}}\Sigma_{t_{ij}}}} \tag{7.11}$$

The terms Λ_{ii} are then bounded above 1.0×10^{-3}, i.e., they are replaced in a differentiable fashion with numbers that are $\geq 1.0 \times 10^{-3}$ using the `posfun` function. In addition, the correlation matrix $\Lambda_{ij}/\sqrt{\Lambda_{t_{ij}}\Lambda_{t_{ij}}}$ is decomposed via a Choleski decomposition, the divisors of which is forced to be > 0.3 in a differentiable fashion using the `posfun` function. The above operations leave a matrix that is sufficiently positive definite and close enough to Σ_1 unchanged.

7.4 Missing data

Missing data points are included into the model as parameters to be estimated. If there are a substantial number of missing data points, this will induce bias into the estimates.

7.5 The likelihood function

The model was fit by maximum-likelihood or, more correctly, by finding the mode of the Bayesian posterior distribution. A robust likelihood function that is a mixture of a normal distribution and a Cauchy distribution is employed. The amount of robustness can be changed by the user.

7.6 Model selection

Model selection consists of fitting the model to the data for various values of the parameters (p, q, r, s) and trying to determine the simplest model that adequately fits the data, if any.

The two criteria which are used for this are the likelihood ratio test and investigation of the residuals in the form of the Box-Ljung statistic. The likelihood-ratio test is used for general model selection, while the Box-Ljung statistic is used to investigate whether or not the model can adequately fit the changes in the covariance matrices Σ_t that occur over time.

7.7 The Box-Ljung statistic

The following Box-Ljung Statistic was employed to test the ability of the model to model the time varying covariance structure of the time series. This statistic is calculated from the estimated standardized residuals z_t, for $t = 1, \ldots n$, where for each t, z_t is an m-dimensional vector. The z_i are obtained in the calculations necessary to calculate the log-likelihood function.

$$\hat{\mu}_j = \frac{1}{n}\sum_{i=1}^{n} z_{ij} \tag{7.12}$$

$$z'_{ij} = z_{ij} - \hat{\mu}_j \tag{7.13}$$

$$\hat{\sigma}_{jk} = \frac{1}{n}\sum_{i=1}^{n} z'_{ij} z'_{ik} \tag{7.14}$$

$$\gamma_{ijk} = \frac{\frac{1}{n-l}\sum_{i=1}^{n-l}(z'_{ij}z'_{ik} - \hat{\sigma}_{jk})(z'_{i,j+l}z'_{i,k+l} - \hat{\sigma}_{jk})}{\frac{1}{n}\sum_{i=1}^{n}(z'_{ij}z'_{ik} - \hat{\sigma}_{jk})^2} \tag{7.15}$$

Under the null hypothesis that the model is adequate, and if the z_i are normally distributed, then the sum

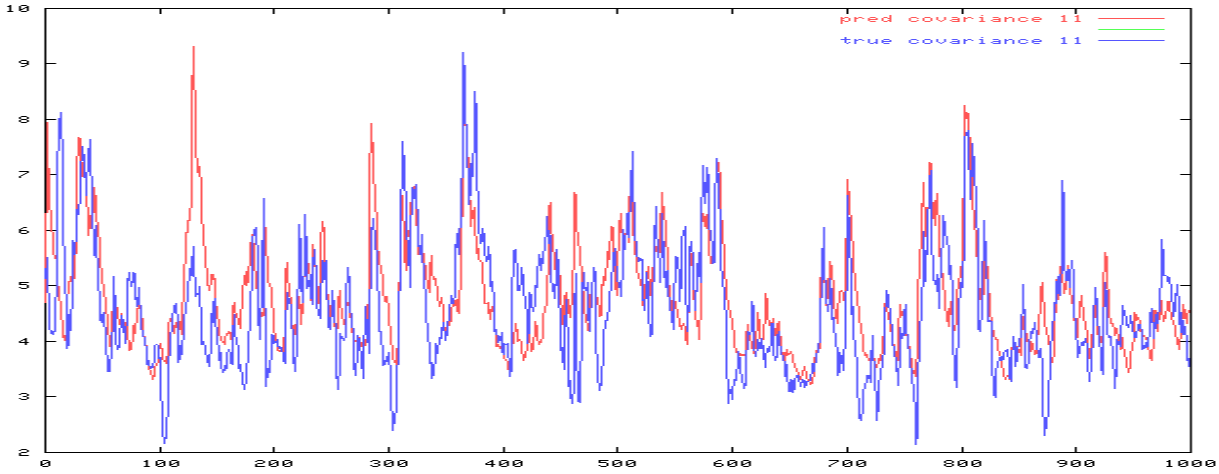
$$LB(K)_{ij} = n\sum_{k=1}^{k} w_k \gamma_{ijk}^2$$

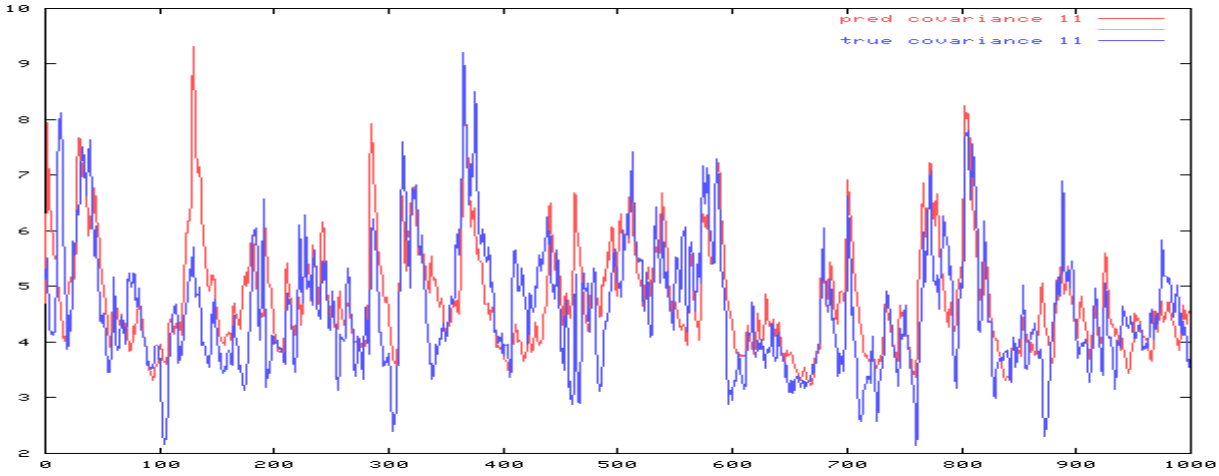
is asymptotically distributed as a χ^2 random variables with K degrees of freedom. Here, $w_k = (n+2)/(n-k)$.

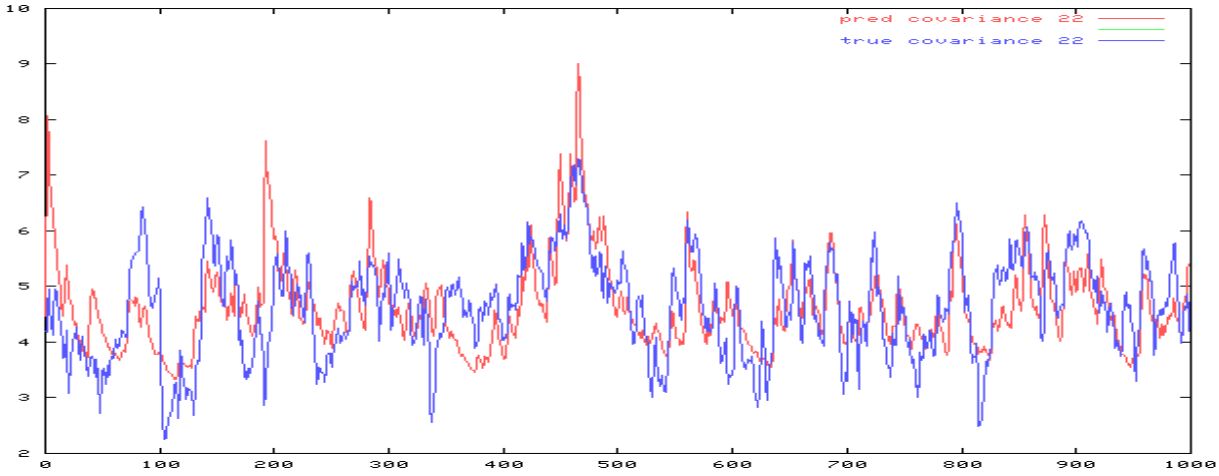
7.8 Analysis of simulated data

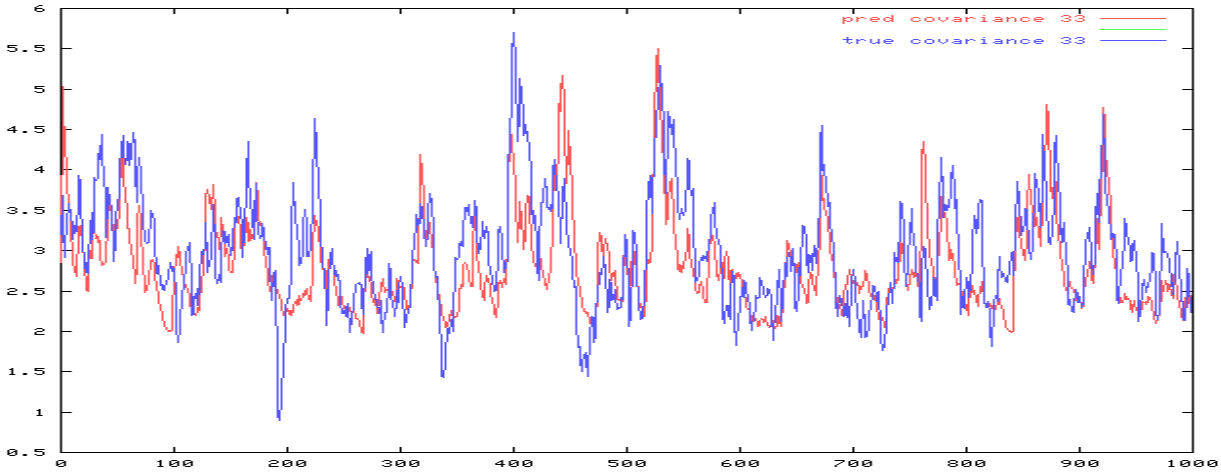
One method to get an idea how well a statistical model works is to use it with simulated data where the true values of the parameters being estimated are known. A simple simulator that can generate data sets is included with the `mgarch` package. The simulator generated a 4-dimensional set of 1,000 observations. A type $1, 1, 1, 1$ process was simulated and analyzed.

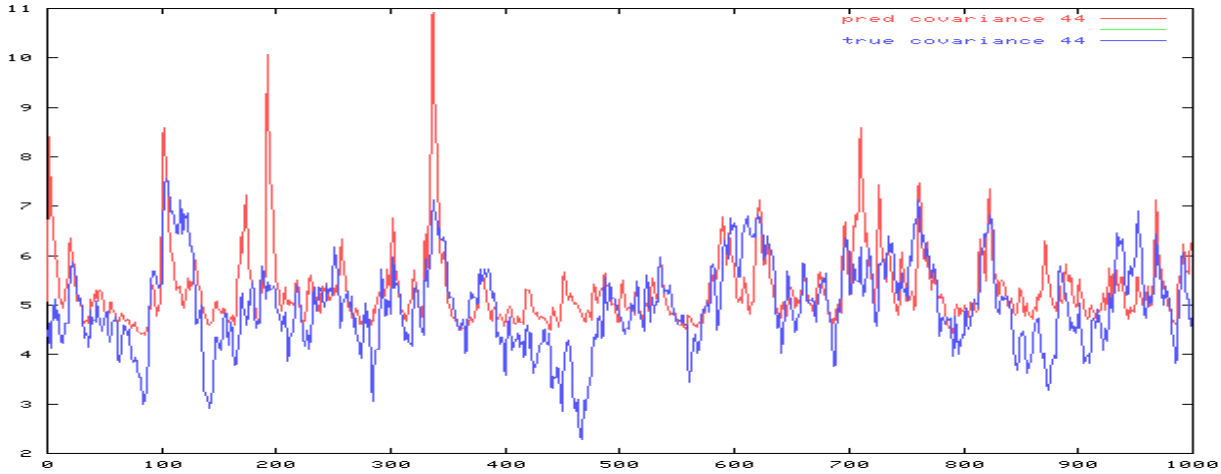
The following plots show the actual and predicted values for the diagonal variance and correlation terms for the analysis with a type $1, 1, 1, 1$ model.

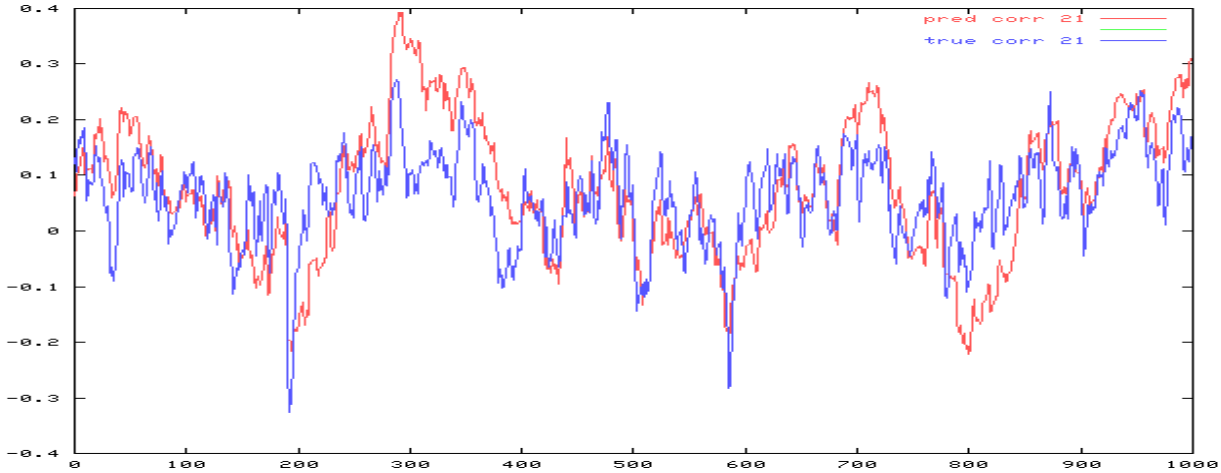

pred covariance 11
true covariance 11
10
9
8
7
6
5
4
3
2
0
100
200
300
400
500
600
700
800
900
1000

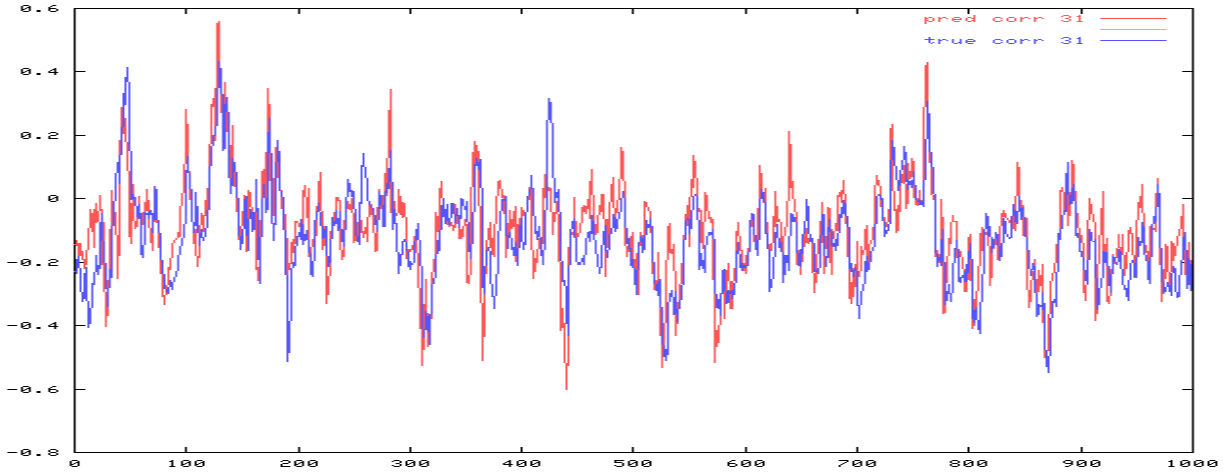

pred covariance 11
true covariance 11
10
9
8
7
6
5
4
3
2
0
100
200
300
400
500
600
700
800
900
1000

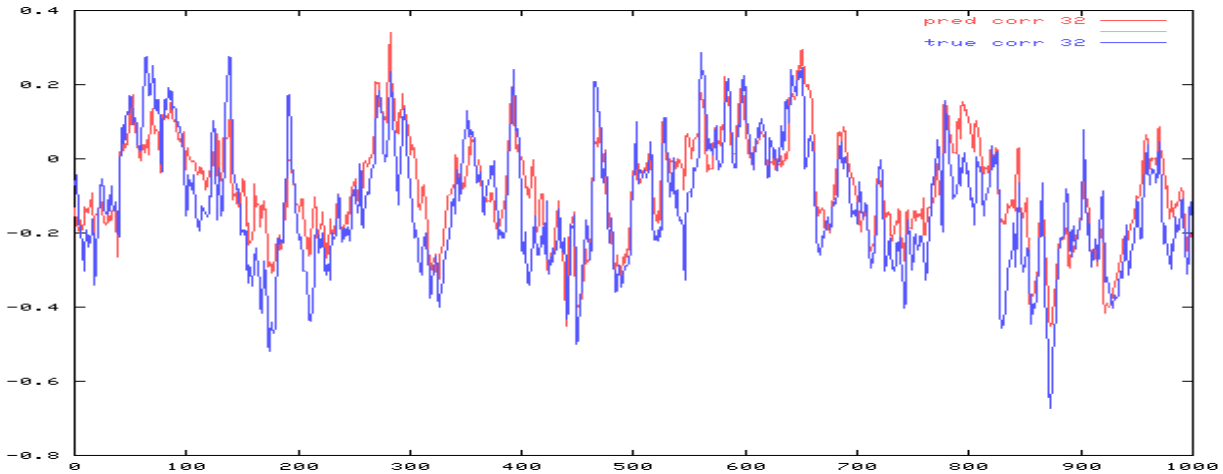

pred covariance 22
true covariance 22
10
9
8
7
6
5
4
3
2
0
100
200
300
400
500
600
700
800
900
1000

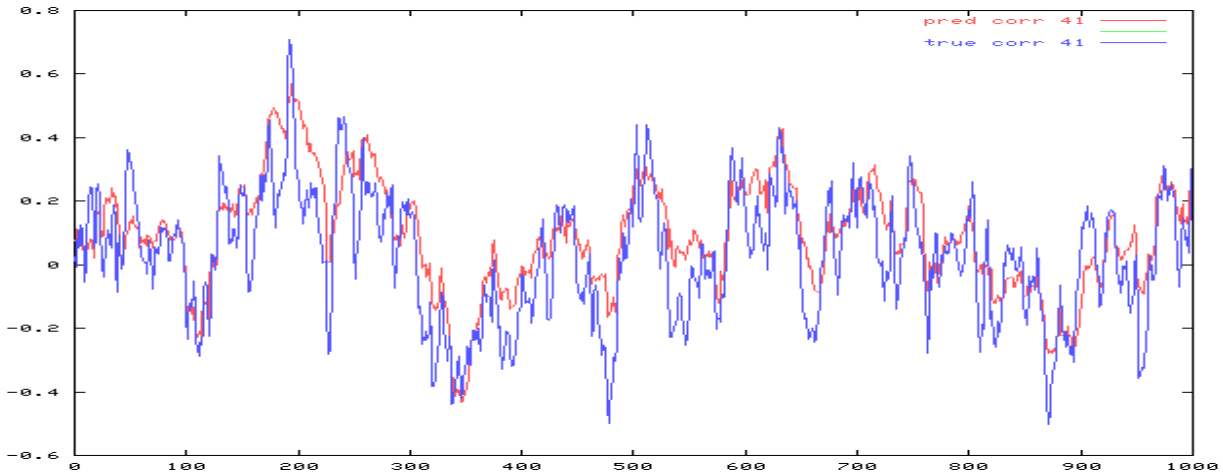

pred covariance 33
true covariance 33
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
100
200
300
400
500
600
700
800
900
1000

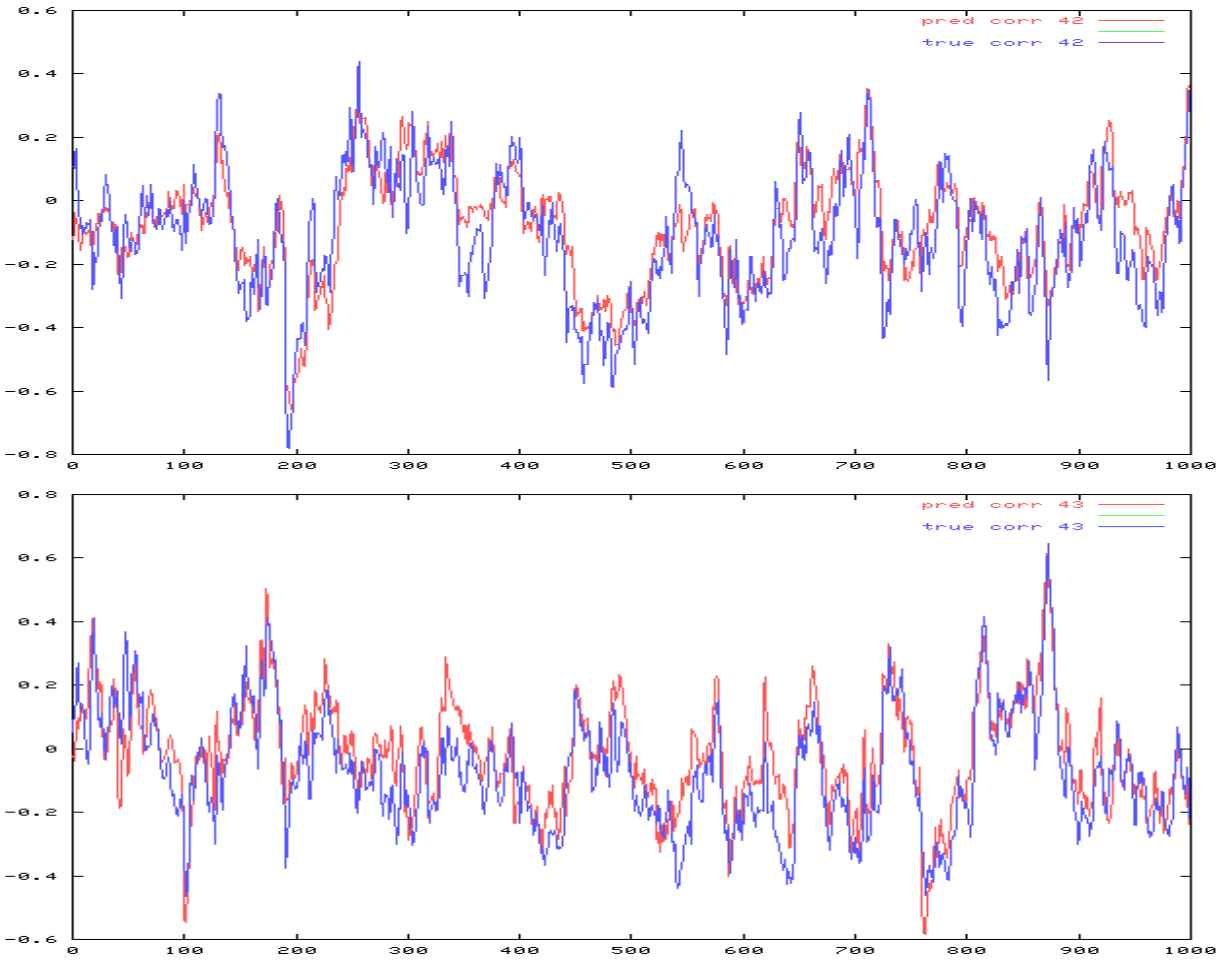

pred covariance 44
true covariance 44
11
10
9
8
7
6
5
4
3
2
0
100
200
300
400
500
600
700
800
900
1000


pred corr 21
true corr 21
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
0
100
200
300
400
500
600
700
800
900
1000


pred corr 31
true corr 31
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
100
200
300
400
500
600
700
800
900
1000


pred corr 32
true corr 32
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
100
200
300
400
500
600
700
800
900
1000


pred corr 41
true corr 41
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
100
200
300
400
500
600
700
800
900
1000



7.9 Analysis of real data

The data consist of daily observations of the German Mark/US Dollar and Japanese Yen/US dollar exchange rates, as well as the SP-500 and Tokyo (TOKYOSE) stock exchange indices. For this data set, $m = 4$, and there were 1301 time periods with 211 missing values.

7.9.1 Model Parameters log-likelihood directory p, q, r, s.

```
VARMA
0,0,0,0   221        -1382.56     000
1,0,0,0   241        -1322.47     100
1,1,0,0   253        -1308.57     110

VARMA with DVEC
0,0,1,1   241        -1050.87
```

```
1,1,2,1  283        -928.518
1,2,1,1  289        -924.755

VARMA with DVECI
1,1,2,1a 287        -887.764
1,2,1,1a 293        -888.531
```

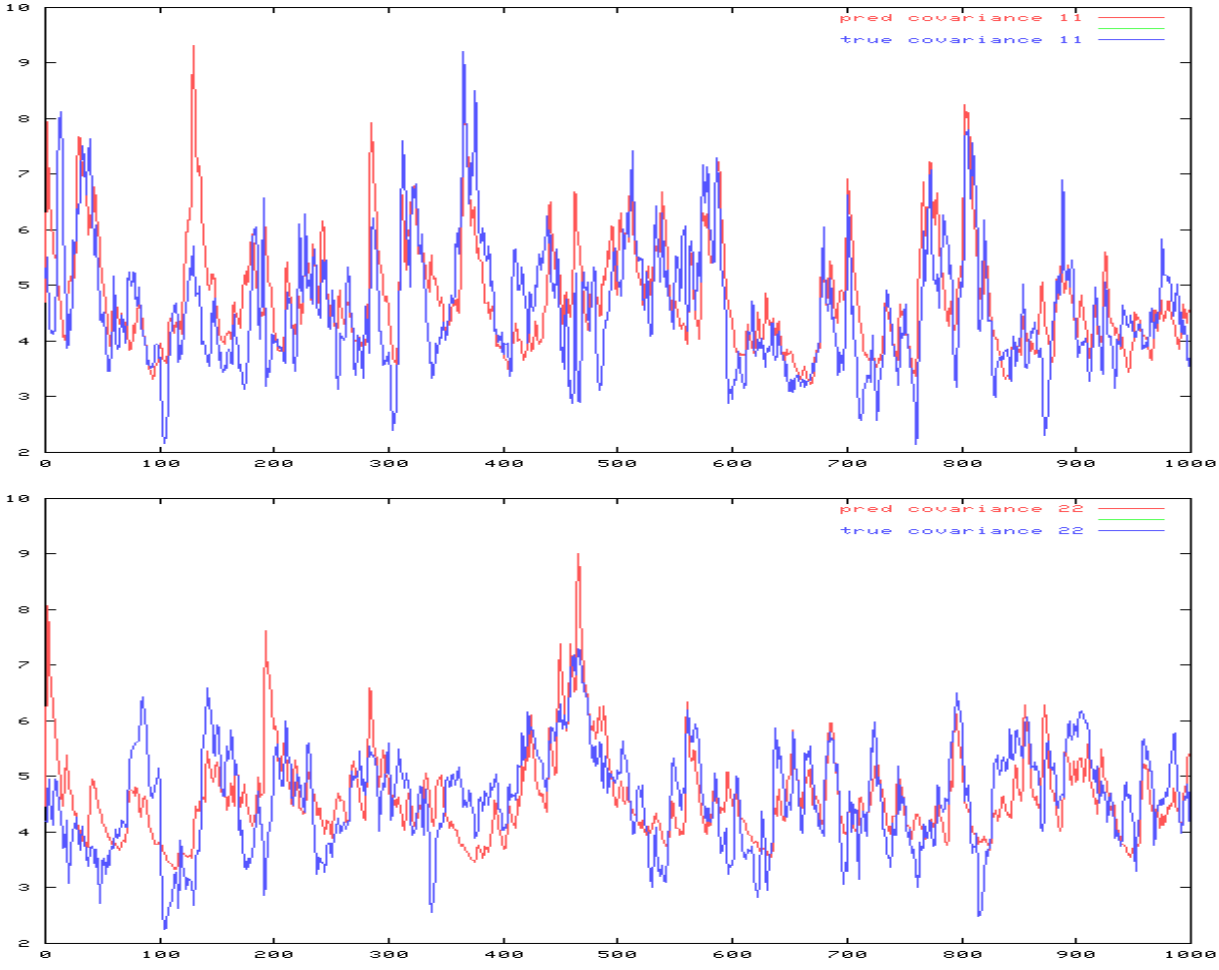
7.9.2 Ljung-Box statistic (chi^2 with 10 degrees of freedom).

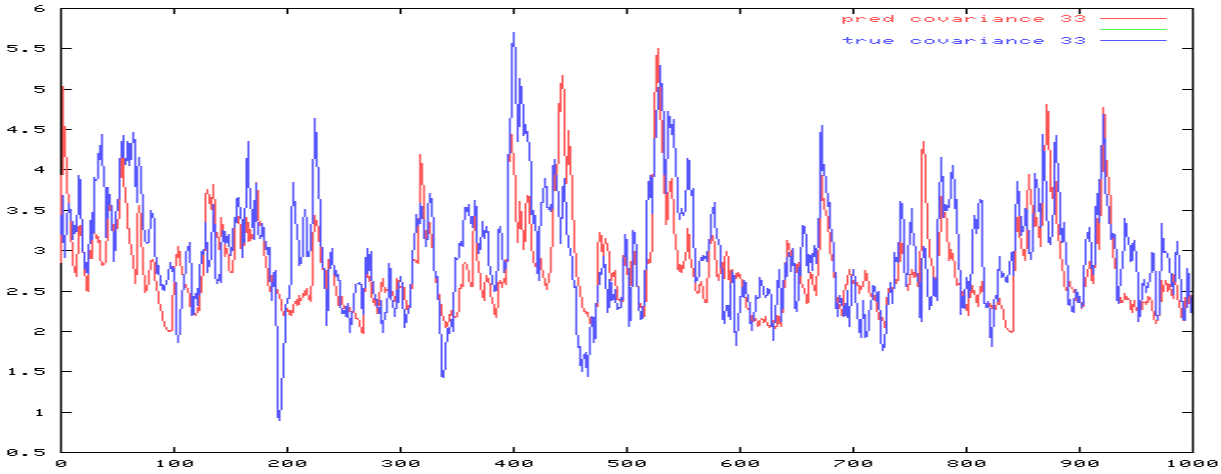
```
VARMA
0,0,0,0        138.953 52.902 26.351 19.171
                52.902 222.502 154.708 59.681
                26.351 154.708 60.328 87.031
                19.171 59.681 87.031 68.889


1,1,0,0        154.977 74.511 19.329 11.472
                74.511 177.016 130.295 59.084
                19.329 130.295 47.499 72.724
                11.472 59.084 72.724 49.329

VARMA with DVEC
0,0,1,1          3.728 13.180 17.682 17.633
                13.180 11.496 25.846 6.016
                17.682 25.846 7.610 6.791
                17.633 6.016 6.791 13.398


1,1,1,1          4.239 9.519 10.866 10.885
                 9.519 6.434 21.734 8.047
                10.866 21.734 4.089 8.318
                10.885 8.047 8.318 12.814

1,2,1,1          5.660 10.348 11.029 11.557
                10.348 7.011 21.727 7.039
                11.029 21.727 4.819 7.908
                11.557 7.039 7.908 10.684

1,1,2,1          6.920 11.698 11.464 12.593
                11.698 4.914 24.677 8.179
                11.464 24.677 2.399 8.855
                12.593 8.179 8.855 10.985
```

```
VARMA with DVECI
1,2,1,1a          4.352  9.658  9.402  8.542
                  9.658  7.646 17.516  8.4160
                  9.402 17.516  5.795  7.108
                  8.542  8.416  7.108 10.483

1,1,2,1a          4.785 17.077  8.760 10.487
                 17.077  6.718 18.563  9.736
                  8.760 18.563  3.270  8.525
                 10.487  9.736  8.525 10.253
```

While the model $1,1,2,1a$ produced almost as high a log-likelihood value as model $1,2,1,1a$, the superior performance of the latter model with respect to the Box-Ljung statistic might prompt us to consider it the model of choice.

The following plots show the actual and predicted values for the diagonal variance and correlation terms.




pred covariance 33
true covariance 33
6
5.5
5
4.5
4
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3
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2
1.5
1
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100
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300
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500
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700
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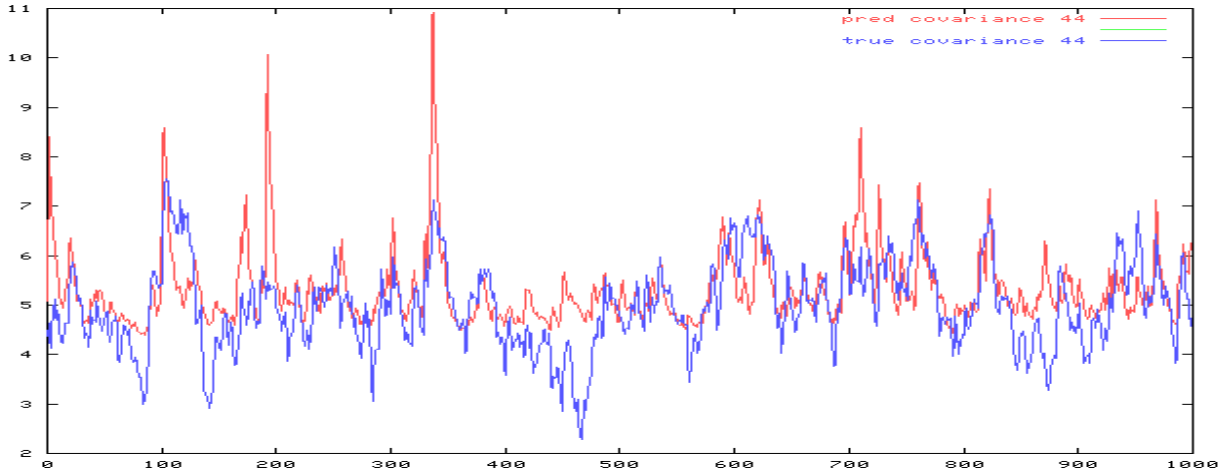
900
1000


pred covariance 44
true covariance 44
11
10
9
8
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6
5
4
3
2
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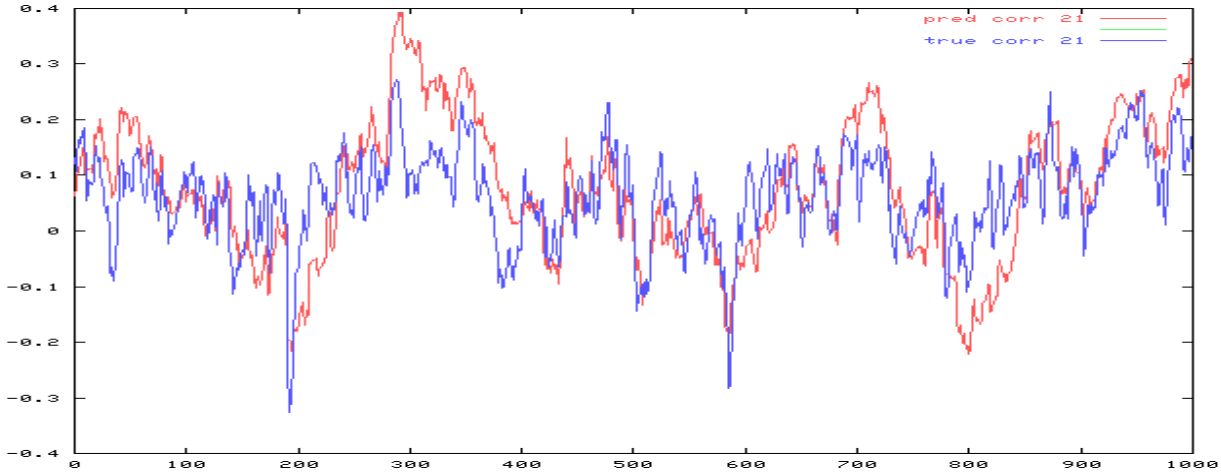
pred corr 21
true corr 21
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
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100
200
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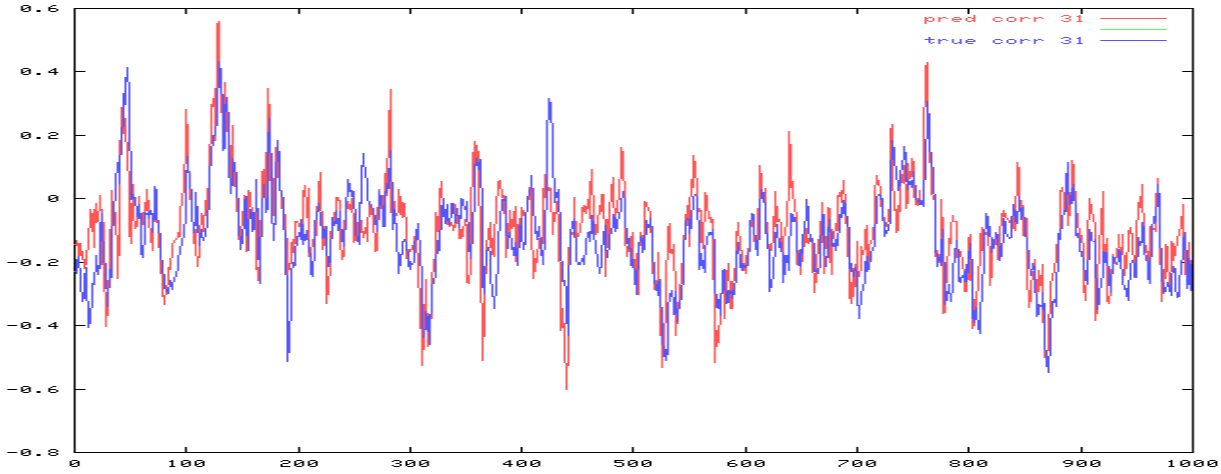
pred corr 31
true corr 31
0.6
0.4
0.2
0
-0.2
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-0.6
-0.8
0
100
200
300
400
500
600
700
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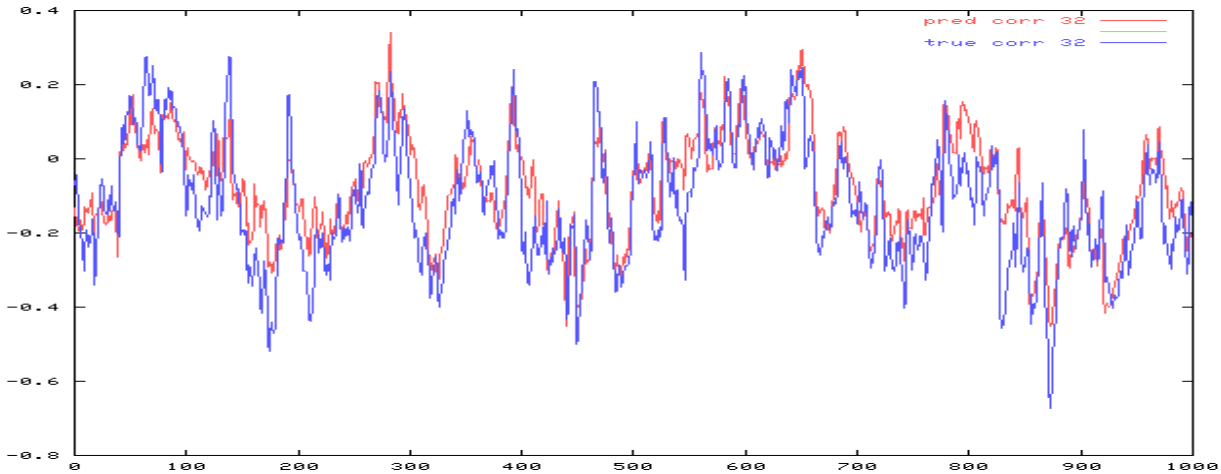
900
1000


pred corr 32
true corr 32
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
100
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700
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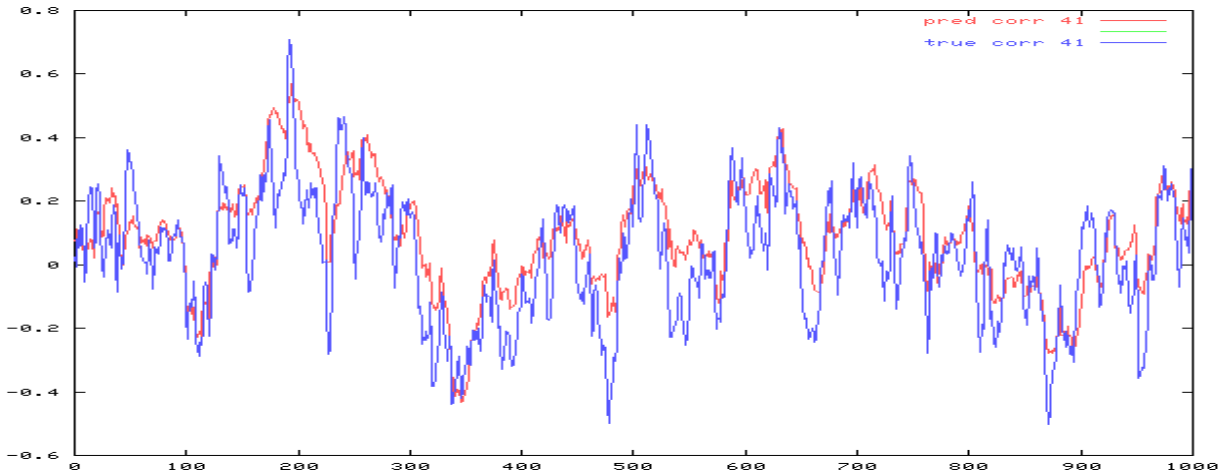
pred corr 41
true corr 41
0.8
0.6
0.4
0.2
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-0.2
-0.4
-0.6
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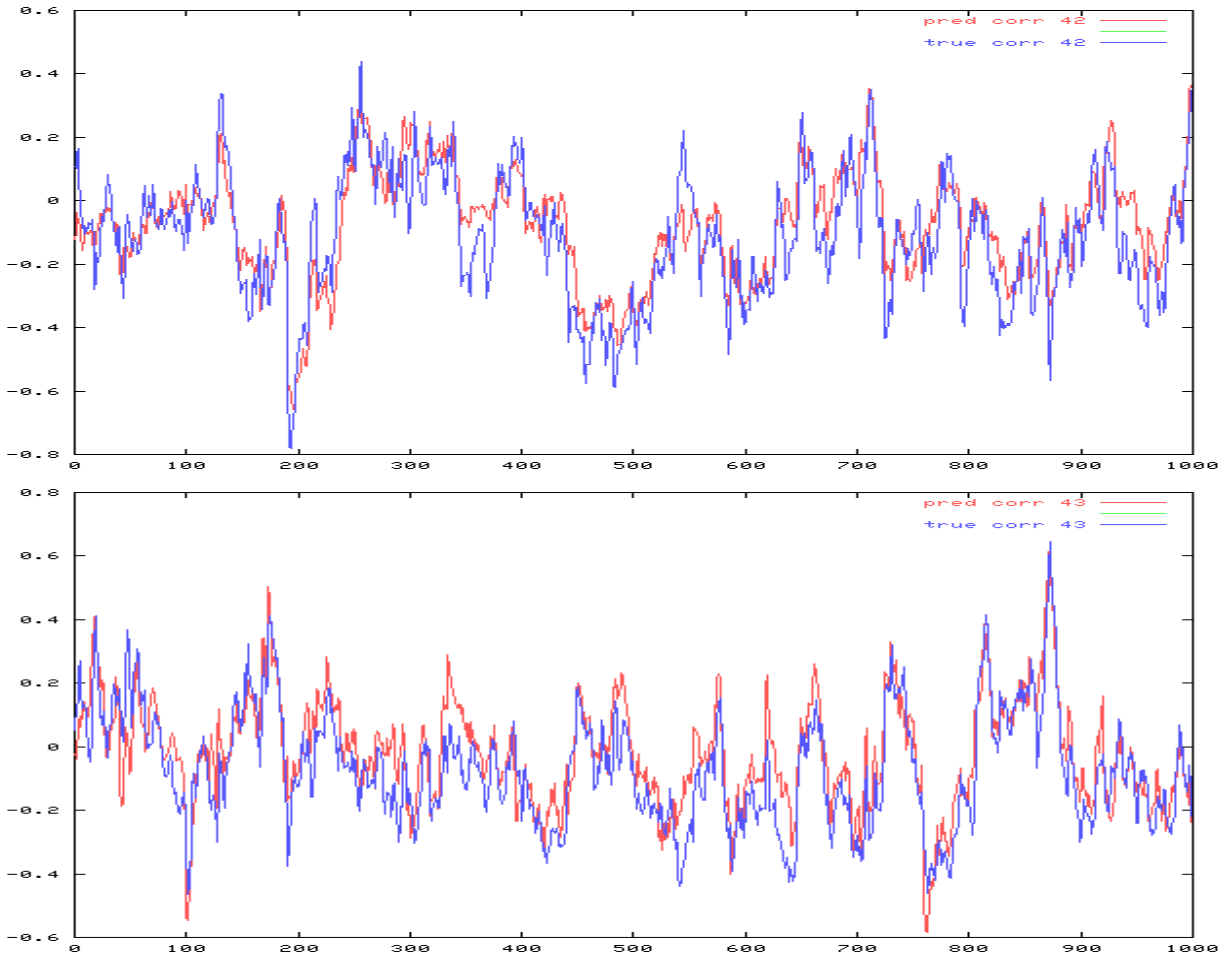

7.10 Input format

By default, the stand-alone version of the model attempts to read in the data from a file named `mgarch.dat`. This can be changed by a command line option. A reasonable command line option would be:

```
mgarch -ind datafile -nox -nohess
```

The command

```
mgarch -?
```

will print out a list of command line options.

Part of a data file is shown below. The first line describes the data and specifies the form of the model. The `delta` flag determines whether or not the parameters that measure asymmetric response in the ARCH component of the model are estimated. The robustness number controls the amount of robustness in the likelihood function. A value between 0.0 and 0.5 is probably appropriate. A value of 10,000 is used to indicate missing values in the data.

```
# number of   dimension   p q r s delta robustness
# observations                    flag
  1301          4         0 0 1 1  0       0
-0.473592    -0.30815    -0.199577    -0.154677
0.140859    -0.256788    -0.823379    -0.947582
-0.80579    -0.833361    2.439394     1.208645
-1.542773    -0.855767    0.469603    -0.433346
10000        10000        1.445218    0.462298
6.014853    4.964597    -0.189343    -0.231408
-1.064758    -1.700819    -3.143447    0.62605
-0.608465    -2.618972    1.641306    2.127487
-5.242424    2.902805    2.60543      -0.668981
2.205787    2.026769    -1.42811    -0.141505
 // ......................................

10000         10000       -1.072871    0.365977
-0.208759    1.51892     -0.59516      -0.029556
-2.413508    -2.578193    2.045828    -0.2362
0.890598    0.119672    -0.415587    0.029485
-2.797967    0.943489    -1.377787    0.283592
1.405865    1.915963    -0.696567    0.450668
10000        10000       -0.31709    0.255885
2.971906    -1.704494    0.835319    0.286408
-3.451449    1.233715    -1.144007    -0.322157
1.342827    0.376409    0.279213    0.226602
```

7.11 Output files

Since the model produces a lot of output, it is a good idea to run it in its own directory, so files can be easily deleted. The independent variables of the optimization are in a file named `mgarch.par`. (`mgarch.bar` is an equivalent binary file.) A more user-friendly report is in the file `mgarch.rep`. The estimated covariances and correlations are in files named `covar.XX` and `correl.XX`.

The model selection criteria have identified the model 1.1.1a as the best of the models considered for these data.

Some parameters of interest are:

```
# alpha:
 0.394461 0.538978 1.19337 0.969918
# A1:
 -0.0531276 0.772529 -0.187692 -0.131215
 0.0898897 -0.399746 -0.142294 -0.106079
```

```
 0.0740065 0.248345 -0.0629680 -0.212928
 0.0918460 -0.0575289 -0.0700786 0.0537302
# B1:
 -0.00719450 -0.344793 0.115020 0.00516664
 -0.0943230 0.474330 0.147845 0.0936166
 -0.0860047 -0.243294 0.0187986 0.217280
 -0.0815394 0.0843289 0.00782384 -0.0539808
# F:
 -0.109526 -0.0292127 -0.122395 0.0548869
 0.000332929 -0.0964482 0.0153865 -0.0346829
 -0.0148848 -0.0146167 -0.117961 -0.0529385
 -0.00504663 -0.000547068 0.00413882 -0.133956
# G:
 0.930026 -0.269741 0.136401 0.427047
 -0.0345549 -0.981606 0.00281003 -0.00411475
 0.0976783 -0.0132467 -0.976596 0.0306139
 0.117971 -0.0134465 0.00647385 -0.955173
```

For the four parameters α_i, a value < 1 indicates that negative values seem to have a larger effect on changes in the covariance structure than do positive ones. This effect seems to be much larger in the dollar cross rates than in the stock exchanges indices.

7.12 The code for the BEKKGARCH model

The code for the BEKKGARCH model follows. Additional comments have been added to the code.

```
DATA_SECTION
  // This section describes the data inputs to the model.
  // By default they are read in from the file bekkgarch.dat.
  init_int na // number of time periods
  init_int m  // dimension of the vector time series
  init_int p  // degree of autoregression must be >=0
  init_int q  // degree of moving average mult be >=0
  init_int ra  // degree of arch must be>=0
  init_int sg  // degree of arch must be>=0
  init_int delta_switch // turns on asymmetric response to shocks
  init_number robustness // amount of robustness probably something
             // between 0 and .05 is right
  int n
  int msquared
 !! n=na-p; // number of obs for conditional likelihood
  init_matrix cY(-p+1,n,1,m) // the vector time series of observations
```

```
 int nmiss
LOC_CALCS
 msquared=m*m;
 int ii=0;
 int j;
 int i;
 for (i=-p+1;i<=n;i++)
   for (j=1;j<=m;j++)
     if (cY(i,j)==10000) ii++;
 nmiss=ii;
END_CALCS
 ivector rowmiss(1,nmiss)
 ivector colmiss(1,nmiss)
LOC_CALCS
 ii=1;
 for (i=1;i<=n;i++)
   for (j=1;j<=m;j++)
     if (cY(i,j)==10000) {
       rowmiss(ii)=i;
       colmiss(ii)=j;
       ii++;
     }
END_CALCS
 int m1
 int beginSigma
 matrix Idm(1,m,1,m)
 ivector beginF(1,ra)
 ivector beginG(1,sg)
 ivector beginA(1,p)
 ivector beginB(1,q)
 int nstart
LOC_CALCS
 nstart=0;
 if (nmiss>0) nstart=1;
 m1=m*(m+1)/2; // "size" of n x n symmetric matrix
 Idm=identity_matrix(1,m);
 if (p) beginA.fill_seqadd(1+nstart,1);
 if (q) beginB.fill_seqadd(p+1+nstart,1);
 if (ra) beginF.fill_seqadd(p+q+1+nstart,1);
 if (sg) beginG.fill_seqadd(p+q+1+nstart,1);
 beginSigma=p+q+1+nstart;
END_CALCS
```

```
PARAMETER_SECTION
 LOC_CALCS
  int mm=m;
  int dstart;
  if (delta_switch>0)
    dstart=p+q+2+nstart;
  else
    dstart=-1;
 END_CALCS
  // the initial values for the time series and disturbance as
  // estimated parameters
  init_bounded_vector mudev(1,m,-100,100,-1)
  init_bounded_vector delta(1,m,.1,1.9,dstart)
  vector mu(1,m)
  vector esd(1,m)
  vector muemp(1,m) // empirical covariance matrix
  matrix Y(-p+1,n,1,m) // the vector time series of observations
  init_matrix_vector A1(1,p,1,mm,1,mm,beginA) // pars for the AR coff matrices
  3darray A(1,p,1,m,1,m) // pars for the AR coff matrices
  init_matrix_vector B1(1,q,1,mm,1,mm,beginB) // pars for the MA coff matrices
  3darray B(0,q,1,m,1,m) // has the additional B(0)=Id
  3darray Bt(0,q,1,m,1,m) // has the additional B(0)=Id
  4darray cov(1,n,0,q,1,m,1,m) // the m x m blocks for the covariance
  3darray TB_S(0,q,1,m,1,m)
  matrix Omega(1,m,1,m)
  3darray B_S(0,q,1,m,1,m)
  init_bounded_vector v_Sigma(1,m1,-10,10.1,beginSigma); // pars for Sigma
  matrix Semp(1,m,1,m)
  matrix SSemp(1,m,1,m)
  matrix ch_Sigma(1,m,1,m)
  init_bounded_vector_vector Fcoff(1,ra,1,msquared,-1.000,1.0,beginF)
  3darray F(1,ra,1,m,1,m)
  3darray tF(1,ra,1,m,1,m)
  init_bounded_vector_vector Gcoff(1,sg,1,msquared,-.98,.98,beginG)
 LOC_CALCS
  if (ra)
  {
    int mmin,mmax;
    mmin=Fcoff(1).indexmin();
    mmax=Fcoff(1).indexmax();
    for (int ij=mmin;ij<=mmax;ij++) if (value(Fcoff(1)(ij))==0.0)
      Fcoff(1)(ij)=0.02;
```

```
  }
  if (sg)
  {
    int mmin,mmax;
    mmin=Gcoff(1).indexmin();
    mmax=Gcoff(1).indexmax();
    for (int ij=mmin;ij<=mmax;ij++) if (value(Gcoff(1)(ij))==0.0)
      Gcoff(1)(ij)=0.001;
  }
 END_CALCS
  3darray G(1,sg,1,m,1,m)
  3darray tG(1,sg,1,m,1,m)
  3darray Sigma(1,n,1,m,1,m)
  init_bounded_vector missvals(1,nmiss,-5.0,5.0);
  vector arpart(1,m)
  matrix r(1,n,1,m)
  3darray rr(1,n,1,m,1,m)
  vector vecr(1,n*m) // VEC[r]
  vector y(1,n*m)
  number ldet
  objective_function_value f
  matrix Yv(-p+1,n,1,m) // after subtracting off the mean
 !! int q1m=(q+1)*m;
 !!CLASS banded_symmetric_dvar_matrix S(1,n*m,q1m);
PROCEDURE_SECTION
  int t; int i; int j;
  fill_matrices_with_independent_parameters();
  Y=cY;
  add_missing_values();
  calculate_time_series_mean();
  calculate_the_residuals();
  calculate_the_empirical_covariance();
  SSemp=get_initial_sigma();
  dvariable fpen=calculate_the_sub_variances_BEKK();
  calculate_the_sub_covariances();
  calculate_the_covariance_matrix();
  int ierr=0;
  // choleski decomposition of a banded symmetric matrix
  // produces a banded lower triangular matrix
  dvariable fpen1=0.0;
  banded_lower_triangular_dvar_matrix blt=choleski_decomp_positive(S,
    1.e-6,fpen1);
```

```
  fpen+=fpen1;
  // solve for y=inv(blt)*vecr
  y=solve(blt,vecr);
  int ss=0;
  dvariable lno=ln_det(Sigma(1),ss);
  f+=norm2(log(delta));
  for (i=1;i<=q;i++) f+=norm2(B1(i));
  f+=norm2(v_Sigma);
  for (i=1;i<=ra;i++) f+=norm2(F(i));
  for (i=1;i<=sg;i++) f+=norm2(G(i));
  dvariable lndet=0.0;
  for (i=1;i<=n*m;i++) lndet+=log(blt(i,i));
  // robust log-likelihood function -- mixture of normal and
  // tiny bit of cauchy
  dvar_vector y2= square(y);
  if (robustness>1.e-20)
    f+= lndet - sum(log(mfexp(-0.5*y2)+robustness/(1.0+y2)));
  else
    f+= lndet - sum(log(mfexp(-0.5*y2)+.0001/(1.0+y2)));

  f+=fpen;
  (*ad_printf)("f = %lf\n",value(f));
FUNCTION fill_matrices_with_independent_parameters
  int ii=1; int i=1; int iii;
  double d=sqrt(0.1);
  if  (!sg) d=1.0;
  ch_Sigma.initialize();
  // this is the choleski decomp parameterization of the
  // covariance matrix
  for (i=1;i<=m;i++)
    for (int j=1;j<=i;j++) {
      if (i==j)ch_Sigma(i,i)+=d;
      ch_Sigma(i,j)+=v_Sigma(ii++);
    }
  for (iii=1;iii<=ra;iii++) {
    if (iii==1 || active(Fcoff(iii))) {
      ii=1;
      F(iii).initialize();
      tF(iii).initialize();
      for (i=1;i<=m;i++) {
        for (int j=1;j<=m;j++)
          F(iii)(i,j)=Fcoff(iii)(ii++);
```

```
      }
    }
    tF(iii)=trans(F(iii));
  }

  for (iii=1;iii<=sg;iii++) {
    if (iii==1 || active(Gcoff(iii))) {
      ii=1;
      G(iii).initialize();
      tG(iii).initialize();
      for (i=1;i<=m;i++) {
        for (int j=1;j<=m;j++) {
          G(iii)(i,j)=Gcoff(iii)(ii++);
        }
        if (iii==1) G(iii)(i,i)+=0.90;
      }
    }
    tG(iii)=trans(G(iii));
  }
  B.initialize();
  A.initialize();
  // B(0) is the identity matrix
  B(0)=Idm;
  for (i=1;i<=p;i++) A(i)=A1(i);
  for (i=1;i<=q;i++) B(i)=B1(i);
  for (i=0;i<=q;i++) Bt(i)=trans(B(i));

FUNCTION calculate_the_residuals
  int t; int j;
  mu=muemp+mudev;
  for (t=-p+1;t<=0;t++) Yv(t)=Y(t)-mu;
  for (t=1;t<=n;t++) {
    Yv(t)=Y(t)-mu;
    calculate_autoregressive_part(t);
    r(t)=Yv(t)-arpart;
  }
  int ii=0;
  // this corresponds to the VEC operator
  for (int i=1;i<=n;i++)
    for (j=1;j<=m;j++) vecr(++ii)=r(i,j);

FUNCTION void calculate_the_residuals2(dvar_matrix& e)
```

```
  int t; int j;
  mu=muemp+mudev;
  for (t=-p+1;t<=0;t++) Yv(t)=Y(t)-mu;
  for (t=1;t<=n;t++) {
    Yv(t)=Y(t)-mu;
    calculate_autoregressive_part(t);
    e(t)=Yv(t)-arpart;
    for (j=1;j<=q;j++) {
      if (t<=j) break;
      e(t)-=B(j)*e(t-j);
    }
  }

FUNCTION calculate_the_sub_covariances
  int i; int k; int l;
  int qq=0;
  for ( l=1;l<=q;l++) {
    if (!active(B1(l))) break;
    qq=l;
  }
  cov.initialize();
  for (i=1;i<=n;i++) {
    for (int l=0;l<=qq;l++) {
      if (i<=l) break;
      for (int k=0;k<=qq-l;k++) {
        int ilk=i-l-k;
        if (ilk<1) ilk=1;
        cov(i,l)+=B(l+k)*Sigma(ilk)*Bt(k);
      }
    }
  }

FUNCTION calculate_the_empirical_covariance
  int i;
  Semp.initialize();
  ivector sgn(1,m);
  esd.initialize();
  for (i=1;i<=n;i++) {
    esd+=square(r(i));
  }
  esd/=n;
  esd=sqrt(esd);
```

```
  if (active(delta)) {
    dvar_vector mult_neg=elem_div(esd,delta);
    dvar_vector mult_pos=elem_prod(esd,delta);
    for (i=1;i<=n;i++) {
      sgn.initialize();
      dvar_vector sr=sfabs(elem_div(r(i),esd));
      for (int j=1;j<=m;j++)
        if (r(i,j)<0)
          sr(j)=-sr(j)*mult_neg(j);
        else
          sr(j)=sr(j)*mult_pos(j);
      rr(i)=outer_prod(sr,sr);
    }
    Semp=empirical_covariance(r);
  }
  else
  {
    for (i=1;i<=n;i++) {
      rr(i)=outer_prod(r(i),r(i));
      Semp+=rr(i);
    }
    Semp/=n;
  }
  for (int j=1;j<=m;j++)
    esd(j)=sqrt(Semp(j,j));


FUNCTION dvariable calculate_the_sub_variances_diagonal_vector_garch(void)
  int i; int k; int ii; int jj;
  dvar_vector norms(1,n);
  dvariable fpen=0.0;
  dvariable fpen1;
  Omega=ch_Sigma*SSemp*trans(ch_Sigma);
  Sigma.initialize();
  // set the first Sigma equal to the empirical covariance
  int rsmax=mymax(ra,sg);
  Sigma(1)=SSemp;
  //cout << Sigma(1) << endl;
  dvar_matrix SS=scale(Sigma(1),esd);
  //cout << SS << endl;
  fpen+=positivize_sigma(SS);
  //cout << SS << endl;
```

```
dvariable ns=norm(SS);
 norms(1)=ns;
fpen1=0.0;
dvariable bn=mf_upper_bound(ns,1000.0,fpen1);
if (fpen1>0.0) {
  SS*=(bn/ns);
  fpen+=fpen1;
}
Sigma(1)=unscale(SS,esd);
for (i=2;i<=rsmax;i++) {
  Sigma(i)=Sigma(1);
  norms(i)=norms(1);
}

int mmin=Sigma(1).indexmin();
int mmax=Sigma(1).indexmax();
dvar_vector s(mmin,mmax);
for (i=rsmax+1;i<=n;i++) {
  Sigma(i)=Omega;
  if (ra) Sigma(i)+=elem_prod(F(1),rr(i-1));
  for (ii=2;ii<=ra;ii++) {
    if (active(Fcoff(ii)))
      Sigma(i)+=elem_prod(F(ii),rr(i-ii));
  }

  if (sg) Sigma(i)+=elem_prod(G(1),Sigma(i-1));
  for (ii=2;ii<=sg;ii++) {
    if (active(Gcoff(ii)))
      Sigma(i)+=elem_prod(G(ii),Sigma(i-ii));
  }

  // "positivize" the
  // correlation matrix
  dvar_matrix SS=scale(Sigma(i),esd);
  fpen+=positivize_sigma(SS);
  dvariable ns=norm(SS);
  norms(i)=ns;
  fpen1=0.0;
  dvariable bn=mf_upper_bound(ns,1000.0,fpen1);
  if (fpen1>0.0) {
    SS*=(bn/ns);
    fpen+=fpen1;
```

```
    }
    Sigma(i)=unscale(SS,esd);
  }
  dvector trend(1,n);
  trend.fill_seqadd(-1,2.0/(n-1));
  cout << "norms*trend/norm(norms)" << endl;
  dvariable npen=norms*trend/norm(norms);
  cout << norms*trend/norm(norms) << endl;
  fpen+=npen;
  if (fpen>1.0)
    cout << " fpen = " << fpen << endl;
  return fpen;

FUNCTION dvariable calculate_the_sub_variances_BEKK(void)
  int i; int k; int ii; int jj;
  dvar_vector norms(1,n);
  dvariable fpen=0.0;
  dvariable fpen1;
  Omega=ch_Sigma*SSemp*trans(ch_Sigma);
  Sigma.initialize();
  // set the first Sigma equal to the empirical covariance
  int rsmax=mymax(ra,sg);
  Sigma(1)=SSemp;
  dvar_matrix SS=scale(Sigma(1),esd);
  fpen+=positivize_sigma(SS);
  dvariable ns=norm(SS);
   norms(1)=ns;
  fpen1=0.0;
  dvariable bn=mf_upper_bound(ns,1000.0,fpen1);
  if (fpen1>0.0) {
    SS*=(bn/ns);
    fpen+=fpen1;
  }
  Sigma(1)=unscale(SS,esd);
  for (i=2;i<=rsmax;i++) {
    Sigma(i)=Sigma(1);
    norms(i)=norms(1);
  }

  int mmin=Sigma(1).indexmin();
  int mmax=Sigma(1).indexmax();
  dvar_vector s(mmin,mmax);
```

```
for (i=rsmax+1;i<=n;i++) {
  Sigma(i)=Omega;
  if (ra) Sigma(i)+=F(1)*rr(i-1)*tF(1);
  for (ii=2;ii<=ra;ii++) {
    if (active(Fcoff(ii)))
      Sigma(i)+=F(ii)*rr(i-ii)*tF(ii);
  }

  if (sg) Sigma(i)+=G(1)*Sigma(i-1)*tG(1);
  for (ii=2;ii<=sg;ii++) {
    if (active(Gcoff(ii)))
      Sigma(i)+=G(ii)*Sigma(i-ii)*tG(ii);
  }

  // "positivize" the
  // correlation matrix
  dvar_matrix SS=scale(Sigma(i),esd);
  fpen+=positivize_sigma(SS);
  dvariable ns=norm(SS);
  norms(i)=ns;
  fpen1=0.0;
  dvariable bn=mf_upper_bound(ns,1000.0,fpen1);
  if (fpen1>0.0) {
    SS*=(bn/ns);
    fpen+=fpen1;
  }
  Sigma(i)=unscale(SS,esd);
}
dvector trend(1,n);
trend.fill_seqadd(-1,2.0/(n-1));
cout << "norms*trend/norm(norms)" << endl;
dvariable npen=norms*trend/norm(norms);
cout << norms*trend/norm(norms) << endl;
fpen+=npen;
if (fpen>1.0)
  cout << " fpen = " << fpen << endl;
{
  //ofstream ofs("sigma");

  //for (int i=1;i<=n;i++)
    //ofs << Sigma(i) << endl << endl;
}
```

```
  return fpen;

FUNCTION dvar_matrix scale(dvar_matrix& M,dvar_vector& sd)
   int mmin=sd.indexmin();
   int mmax=sd.indexmax();
   dvar_matrix SM(mmin,mmax,mmin,mmax);
   for (int i=mmin;i<=mmax;i++)
     for (int j=mmin;j<=mmax;j++)
       SM(i,j)=M(i,j)/(sd(i)*sd(j));
   return SM;

FUNCTION dvar_matrix unscale(dvar_matrix& M,dvar_vector& sd)
   int mmin=sd.indexmin();
   int mmax=sd.indexmax();
   dvar_matrix SM(mmin,mmax,mmin,mmax);
   for (int i=mmin;i<=mmax;i++)
     for (int j=mmin;j<=mmax;j++)
       SM(i,j)=M(i,j)*(sd(i)*sd(j));
   return SM;

FUNCTION dvar_matrix get_initial_sigma(void)
   int i,j,k,l,ll,m2,r,s;
   m2=m*m;
   dvar_matrix M(1,m2,1,m2);

   dvar_vector v=VEC(Semp);
   M=identity_matrix(1,m2);
   for (ll=1;ll<=q;ll++)
   {
     for (i=1;i<=m;i++)
     {
       for (j=1;j<=m;j++)
       {
         int col=(i-1)*m+j;
         for (r=1;r<=m;r++)
         {
           for (s=1;s<=m;s++)
           {
             int row=(r-1)*m+s;
             M(row,col)+=B(ll)(r,i)*B(ll)(s,j);
           }
         }
```

```
      }
     }
   }
   v=solve(M,v);
   dvar_matrix tmp= MAT(v,m,m);
   return tmp;

FUNCTION calculate_the_covariance_matrix
  int ioffset; int joffset; int i1; int i; int j1;
  int k; int l;
  int qq=0;
  for ( l=1;l<=q;l++) {
    if (!active(B1(l))) break;
    qq=l;
  }
  S.initialize();
  for (i=1;i<=n;i++) {
    ioffset=(i-1)*m;
    for (int k=0;k<=qq;k++) {
      //if (k>0 && !active(B1)) break;
      joffset=(i-k-1)*m;
      if (joffset<0) break;
      for (i1=1;i1<=m;i1++) {
        int up;
        if (k==0)
          up=i1;
        else
          up=m;
        for (j1=1;j1<=up;j1++) {
          int i2=i1+ioffset;
          int j2=j1+joffset;
          S(i1+ioffset,j1+joffset)=cov(i,k,i1,j1);
        }
      }
    }
    if (S(1,1) < 0)
      cout << S(1,1) << endl;
  }

FUNCTION void calculate_autoregressive_part(int t)
  // The user can put in any (nonlinear) function desired here
  arpart.initialize();
```

```
  for (int j=1;j<=p;j++) arpart+=A(j)*Yv(t-j);

REPORT_SECTION
  int i; int ii; int jj, t;
  for (ii=1;ii<=m;ii++)
  {
    for (jj=1;jj<=ii;jj++)
    {
      ofstream ofs((char*)("covar." + str(ii) +str(jj)));
      ofstream ofs1((char*)("correl." + str(ii) +str(jj)));
      dvar_matrix Covariance(1,m,1,m);
      for (i=1;i<=n;i++) {
        Covariance=Sigma(i);
        for(int j=1;j<=q;j++)
          if ( (i-j)>0 ) Covariance+=B(j)*Sigma(i-j)*trans(B(j));
        ofs << Covariance(ii,jj) << endl;
        ofs1 << Covariance(ii,jj)/
          sqrt(Covariance(ii,ii)*Covariance(jj,jj))<< endl;
      }
    }
  }

  {
    dvar_matrix ymat=MAT(y,n,m);
    for (int i=1;i<=m;i++) {
       ofstream ofs1((char*)("yres." + str(i)));
       dvector tmp(1,n);
       for (t=1;t<=n;t++)
         tmp(t)=value(ymat(t,i));
       ivector hist=histogram(-20,20,81,tmp);
         ofs1 << column_print(hist) << endl;
    }
  }
  report << "The means" << endl;
  report << mu << endl;
  for (i=1;i<=p;i++) {
    report << "A("<< i << ")" << endl;
    report << setfixed() << setprecision(3) << A(i) << endl;
  }
  report << endl;
  for (i=1;i<=q;i++) {
    report << "B("<< i << ")" << endl;
```

```
  report << setfixed() << setprecision(3) << B(i) << endl;
}
report << endl;
report << "delta" << endl;
report << setfixed() << setprecision(3) << delta << endl;
report << endl;
report << "Omega" << endl;
report << setfixed() << setprecision(3) << Omega << endl;
report << endl;
for (i=1;i<=ra;i++) {
  report << "F("<< i << ")" << endl;
  report << setfixed() << setprecision(3) << F(i) << endl;
}
report << endl;
for (i=1;i<=sg;i++) {
  report << "G("<< i << ")" << endl;
  report << setfixed() << setprecision(3) << G(i) << endl;
}
report << endl;
//report << setfixed() << setw(8) << setprecision(1) << S << endl;
{  // calculate predicted observations for next 20 time periods
   // for graphs results are in t.1 t.2 etc
   int npreds=20;
   dvar_matrix e(1,n,1,m);
   calculate_the_residuals2(e);

   dvar_matrix Z(n+1,n+npreds,1,m);
   Z.initialize();

   for (int t=n+1;t<=n+npreds;t++) {
     Z(t)+=mu;
     for (int i=1;i<=p;i++) {
       if (t-i>n)
         Z(t)+=A(i)*(Z(t-i)-mu);
       else
         Z(t)+=A(i)*(Y(t-i)-mu);
     }
     for (i=1;i<=q;i++) {
       if (t-i<=n && t-i>0)
         Z(t)+=B(i)*e(t-i);
     }
   }
```

```
  for (i=1;i<=m;i++) {
    ofstream ofs1((char*)("pred" + str(i)));
    for (t=-p+1;t<=n;t++)
      ofs1 << Y(t,i) << endl;
    for (t=n+1;t<=n+npreds;t++)
      ofs1 << Z(t,i) << endl;
  }
}
dmatrix T(1,m,1,m);
dmatrix chi(1,m,1,m);
T.initialize();
dmatrix Aut(1,m,1,m);
Aut.initialize();
const int K=10;
d3_array gamma(1,K,1,m,1,m);
dmatrix cr(1,n,1,m);
for (i=1;i<=n;i++)
{
  cr(i)=value(y((i-1)*m+1,i*m).shift(1));
  T+=outer_prod(cr(i),cr(i));
}
T=T/n;
for (i=2;i<=n;i++)
{
  Aut+=outer_prod(cr(i-1),cr(i));
}
Aut=Aut/(n-1);
for (i=1;i<=m;i++)
{
  for (int j=1;j<=m;j++)
  {
    Aut(i,j)/=sqrt(T(i,i)*T(j,j));
  }
}
gamma.initialize();
for (int j=1;j<=m;j++)
{
  for (int k=1;k<=m;k++)
  {
    for (int l=1;l<=10;l++)
    {
      double tmp=0;
```

```
        for (i=1;i<=n-l;i++)
        {
          gamma(l,j,k)+=(cr(i,j)*cr(i,k)-T(j,k))*(cr(i+l,j)*cr(i+l,k)-T(j,k));
          tmp+=square(cr(i,j)*cr(i,k)-T(j,k));
        }
        gamma(l,j,k)/=tmp;
      }
    }
  }

  chi.initialize();
  for (int l=1;l<=K;l++)
  {
    chi+=n*(n+2)/(n-l)*square(gamma(l));
  }

  report << "Covariance of standardized residuals" << endl;
  report << T << endl;
  report << "Lag 1 autocorellation of standardized residuals" << endl;
  report << Aut << endl;
  report << "Ljung Box statistic based on chi squared with " << K
         << " degrees of freedom" << endl;
  report << chi << endl;

FUNCTION add_missing_values
  for (int ii=1;ii<=nmiss;ii++) {
    Y(rowmiss(ii),colmiss(ii))=missvals(ii);
  }
  ofstream ofs("testy");
  ofs << Y << endl;

FUNCTION calculate_time_series_mean
  muemp.initialize();
  for (int i=-p+1;i<=n;i++) muemp+=Y(i);
  muemp/=(n+p);

FUNCTION dvariable positivize_sigma(dvar_matrix& TS)
  int ii,jj;
  dvariable fpen=0.0;
  int mmin=TS.indexmin();
  int mmax=TS.indexmax();
  dvar_vector s(mmin,mmax);
```

```
  for (ii=mmin;ii<=mmax;ii++)
    s(ii)=sqrt(posfun(TS(ii,ii),1.e-3,fpen));
  for (ii=mmin;ii<=mmax;ii++)
    for (jj=mmin;jj<=mmax;jj++)
      TS(ii,jj)/=(s(ii)*s(jj));
  TS=positive_definite_matrix(TS,.3,fpen);
  for (ii=mmin;ii<=mmax;ii++)
    for (jj=mmin;jj<=mmax;jj++)
      TS(ii,jj)*=(s(ii)*s(jj));
  return fpen;

GLOBALS_SECTION
  // some C++ compilers don't supply this!
  int mymax(int x,int y)
  {
    if (x>y)
      return x;
    else
      return y;
  }

TOP_OF_MAIN_SECTION

  ofstream ofs("Error.log");
  arrmblsize=5000000;
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(560000);
  gradient_structure::set_CMPDIF_BUFFER_SIZE(15000000);
  gradient_structure::set_MAX_NVAR_OFFSET(1000);
```

Chapter 8

The Kalman Filter

8.1 The Kalman filter

The Kalman filter is a device for estimating parameters in a class of "time-series"-like models that are put into state-space form. We have used the notation from [6], Chapter 3. The general state-space form is an multivariate time series

$$y_t = Z_t \alpha_t + d_t + \epsilon_t$$

where Z_t is an $N \times m$ matrix, d_t is an N-dimensional vector, y_t is an N-dimensional vector, and ϵ_t is a set of serially uncorrelated N-dimensional random vectors with mean 0 and correlation H_t. The elements of α_t are not observable, but are assumed to be generated by a first-order Markov process

$$\alpha_t = T_t \alpha_{t-1} + c_t + R_t \eta_t$$

where T_t is an $m \times m$ matrix, c_t is an $m \times 1$ vector, R_t is an $m \times g$ matrix and η_t is a $g \times 1$ vector of serially uncorrelated random vectors with mean 0 and covariance matrix H_t. The specification of the state-space system is completed by two further assumptions:

1. The initial state vector α_0 has a mean of a_0 and a variance of P_0.
2. The random vectors ϵ_t and η_t are uncorrelated with each other, and uncorrelated with the initial state.

In applications of the model, many of the parameters Z_t, d_t, H_t, T_t, c_t, R_t, and Q_t may be independent of t, in which case we will write them without the subscript. Also, R may be the identity matrix, in which case we will omit it.

As a simple example of such a model, consider the (2-dimensional) random walk observed with error:

$$\begin{aligned} \alpha_t &= \alpha_{t-1} + \eta_t \\ y_t &= \alpha_t + \epsilon_t \end{aligned} \tag{8.1}$$

For this model, the following parameters are fixed

$$T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad R = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad d = (0,0) \quad c = (0,0)$$

while the covariance matrices Q and H are estimated. The true values of Q and H used in the simulation were

$$Q = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix} \quad H = \begin{pmatrix} 3 & -2.5 \\ -2.5 & 3 \end{pmatrix}$$

and the initial value of a is $(0,0)$.

8.2 Equations for the Kalman filter

For a moment, go back to the general state-space model. Given a_0 and P_0, we recursively calculate the a number of quantities via the relationships

$$\begin{aligned} a_{t|t-1} &= T_t\, a_{t-1} + c_t \\ P_{t|t-1} &= T_t\, P_{t-1}\, T_t' + R_t\, Q_t\, R_t' \\ v_t &= y_t - Z_t\, a_{t|t-1} - d_t \\ F_t &= Z_t\, P_{t|t-1}\, Z_t' + H_t \\ a_t &= a_{t|t-1} - P_{t|t-1}\, Z_t'\, F_t^{-1}\, v_t \\ P_t &= P_{t|t-1} - P_{t|t-1}\, Z_t'\, F_t^{-1}\, Z_t\, P_{t|t-1} \end{aligned} \tag{8.2}$$

The log-likelihood function for the models parameters is given by:

$$\log L = -\tfrac{NT}{2} \log 2\pi - 0.5 \sum_{t=1}^{T} \log |F_t| - 0.5 \sum_{t=1}^{T} v_t F_t^{-1} v_t$$

The TPL file for the random walk Kalman filter code follows:

```
DATA_SECTION
  init_int nt
  init_int N
  init_int m
  int m1
  init_matrix Y(1,nt,1,N)
  matrix P0(1,m,1,m)
 !! P0.initialize();
 !! m1=m*(m+1)/2;
PARAMETER_SECTION
  init_bounded_vector Qcoff(1,m1,-10.,10.1)
```

```
  init_bounded_vector Hcoff(1,m1,-10.,10.1)
  init_vector a0(1,m)
  matrix T(1,m,1,m)
  matrix TT(1,m,1,m)
  vector d(1,N)
  vector c(1,m)
  matrix chQ(1,m,1,m)
  sdreport_matrix Q(1,m,1,m)
  matrix chH(1,N,1,N)
  sdreport_matrix H(1,N,1,N)
  matrix Z(1,N,1,m)
  matrix TZ(1,m,1,N)
  objective_function_value f
 LOCAL_CALCS
   d.initialize();
   c.initialize();
   Z.initialize();
   Z(1,1)=1; Z(2,2)=1;
   T.initialize();
   T(1,1)=1; T(2,2)=1;
   TZ=trans(Z);
   TT=trans(T);
PROCEDURE_SECTION
  setup_Q();
  setup_H();
  f+=kalman_filter();
  cout << " f = " << f << endl;

FUNCTION setup_Q
  chQ.initialize();
  int ii=1;
  for (int i=1;i<=m;i++)
    for (int j=1;j<=i;j++)
      chQ(i,j)=Qcoff(ii++);
  Q=chQ*trans(chQ);
FUNCTION setup_H
  chH.initialize();
  int ii=1;
  for (int i=1;i<=N;i++)
    for (int j=1;j<=i;j++)
      chH(i,j)=Hcoff(ii++);
  H=chH*trans(chH);
```

```
FUNCTION dvariable kalman_filter(void)
  dvar3_array P(0,nt,1,m,1,m);
  dvar3_array P1(1,nt,1,m,1,m);
  dvar3_array F(1,nt,1,N,1,N);
  dvar3_array Finv(1,nt,1,N,1,N);
  dvar_matrix Ptemp(1,m,1,m);
  dvar_matrix a(0,nt,1,m);
  dvar_matrix a1(1,nt,1,m);
  dvar_matrix v(1,nt,1,N);
  a(0)=a0;
  P(0)=P0;
  // This is the Kalman filter recursion. The objects tmp1
  // and tmp2 hold common calculations to optimize a bit
  int t;
  for (t=1;t<=nt;t++)
  {
    a1(t)=T*a(t-1)+c;
    P1(t)=T*P(t-1)*TT+Q;
    dvar_vector pred_y=Z*a1(t)+d;
    v(t)=Y(t)-pred_y;
    dvar_matrix tmp1=P1(t)*TZ;
    F(t)=Z*tmp1+H;
    Finv(t)=inv(F(t));
    dvar_matrix tmp2= tmp1*Finv(t);
    P(t)=P1(t)-tmp2*Z*P1(t);
    a(t)=a1(t)+tmp2*v(t);
  }
  int sgn=0;
  dvariable f=0.0;
  for (t=1;t<=nt;t++)
    f+=ln_det(F(t),sgn)+v(t)*Finv(t)*v(t);
  return f;
TOP_OF_MAIN_SECTION
  arrmblsize=20000000;
  gradient_structure::set_CMPDIF_BUFFER_SIZE(3000000);
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(1000000);
```

This example was deliberately not optimized as much as it could be, in order to retain the flavor of the more general state-space problem. For example, since T is the identity matrix and c is the zero vector, the line of code

```
  a1(t)=T*a(t-1)+c;
```

reduces to

```
a1(t)=a(t-1);
```

The parameters being estimated are a_0, Q, and H.

To parameterize the covariance matrices, the Choleski decomposition parameterization was used. This ensures that the covariance matrices are positive (semi-) definite. The technique can be seen in the function `setup_Q`. The lower triangular matrix `ch_Q` is filled with parameters from a bounded vector:

```
FUNCTION setup_Q
  chQ.initialize();
  int ii=1;
  for (int i=1;i<=m;i++)
    for (int j=1;j<=i;j++)
      chQ(i,j)=Qcoff(ii++);
  Q=chQ*trans(chQ); // chQ is the choleski decomposition of Q
```

Notice that the bounded vector `Qcoff` has slightly asymmetric bounds. This is a simple way to ensure that its initial value is not identically zero, which would lead to a singular covariance matrix.

```
  init_bounded_vector Qcoff(1,m1,-10.,10.1)
```

The model parameters, standard deviations, and correlations are reproduced from the standard ADMB report.

index	name	value	std.dev	7	8	9	10	11	12	13	14	15	16
7	a0	-1.1682e+00	9.0191e-01	1.000									
8	a0	1.2218e+00	8.6442e-01	0.352	1.000								
9	Q	9.9468e-01	1.0862e-01	0.059	-0.006	1.000							
10	Q	7.8808e-01	7.8737e-02	0.038	0.028	0.683	1.000						
11	Q	7.8808e-01	7.8737e-02	0.038	0.028	0.683	1.000	1.000					
12	Q	8.7279e-01	9.6118e-02	-0.018	0.069	0.185	0.721	0.721	1.000				
13	H	3.1352e+00	1.8123e-01	-0.015	-0.007	-0.305	-0.136	-0.136	-0.018	1.000			
14	H	-2.7119e+00	1.4922e-01	-0.021	0.001	-0.102	-0.238	-0.238	-0.139	-0.692	1.000		
15	H	-2.7119e+00	1.4922e-01	-0.021	0.001	-0.102	-0.238	-0.238	-0.139	-0.692	1.000	1.000	
16	H	3.2264e+00	1.7936e-01	0.015	-0.029	-0.031	-0.121	-0.121	-0.249	0.370	-0.698	-0.698	1.000

8.3 Parameterizing the covariance matrix parameterizations

The Choleski decomposition parameterization merely ensures that the matrix is positive semi-definite. By adding a small positive number to the diagonal elements, one can ensure that the covariance matrix is positive definite, and can speed up and improve the stability of the estimation. Of course, what is meant by "small" will depend on the particular problem being considered. A modified form of the routine `setup_Q` follows:

```
FUNCTION setup_Q
  int i;
```

```
chQ.initialize();
int ii=1;
for (i=1;i<=m;i++)
  for (int j=1;j<=i;j++)
    chQ(i,j)=Qcoff(ii++);
Q=chQ*trans(chQ); // chQ is the choleski decomposition of Q
for (i=1;i<=m;i++)
  Q(i,i)+=0.1;  // make Q positive definite
```

Performing this modification for the present model for both Q and H causes the program to converge about twice as fast.

Chapter 9

Applying the Laplace Approximation to the Generalized Kalman Filter: with an Application to Stochastic Volatility Models

Let y_i be an N-dimensional multivariate time series for $i = 1, \ldots, n$, where y_i is a random vector with probability density function $p(y_i|\alpha_i)$. For each i, the α_i are random vectors that satisfy the condition

$$\alpha_i = T_i(\alpha_{i-1}, y_{i-1}) + \eta_i \tag{9.1}$$

where $\mu_{\eta_i} = 0$ and $\sigma^2_{\eta_i} = \sigma^2_\eta$.

Let $p(\alpha_1)$ be the probability density function for α_1 before y_1 is observed. After observing y_1, we want to calculate the probability distribution of α_1 given y_1. This is given by

$$p(\alpha_1|y_1) = p(y_1|\alpha_1)\, p(\alpha_1)/p(y_1) \tag{9.2}$$

where

$$p(y_1) = \int_{-\infty}^{\infty} p(y_1|\alpha_1)\, p(\alpha_1)\ \mathrm{d}\alpha_1 \tag{9.3}$$

Let $\phi(y_1, \alpha_1) = \log(p(y_1|\alpha_1)p(\alpha_1))$ and $\hat{\alpha}_1(y_1) = \max_{\alpha_1}\{\phi(y_1, \alpha_1)\}$. Approximate ϕ by its second-order Taylor expansion in α_1 at $\hat{\alpha}_1$.

$$\phi(y_1, \alpha_1) \approx \phi(y_1, \hat{\alpha}_1) + D^2_{\alpha_1\alpha_1}\phi\big(y_1, \hat{\alpha}_1(y_1)\big)\big(\alpha_1 - \hat{\alpha}_1(y), \alpha_1 - \hat{\alpha}_1(y)\big) \tag{9.4}$$

so that

$$p(y) \approx e^{\phi(y_1, \hat{\alpha}_1(y_1))}\int_{-\infty}^{\infty} \exp\left\{ -\Big(- D^2_{\alpha_1\alpha_1}\phi\big(y_1, \hat{\alpha}_1(y_1)\big)\ \big(\alpha_1 - \hat{\alpha}_1(y), \alpha_1 - \hat{\alpha}_1(y)\big)\ \Big)\right\} \mathrm{d}\alpha_1 \tag{9.5}$$

Making a change of variables and integrating, we obtain

$$p(y_1) \approx e^{\phi(y_1, \hat{\alpha}_1(y_1))}(2\pi)^{n/2}\Big| - D^2_{\alpha_1\alpha_1}\phi\big(y_1, \hat{\alpha}_1(y_1)\big)\Big|^{-1/2} \tag{9.6}$$

This is the Laplace approximation to the integral in equation (9.3).

If the distribution of α_1 is (multivariate) normal and the distribution of $y_1|\alpha_1$ is multivariate normal, then $\phi(y_1, \alpha_1)$ is a quadratic function of α_1, so the Laplace approximation is exact. The advantage of the Laplace approximation is that it can be employed for non-normal distributions.

To illustrate this advantage, consider the simple 1-dimensional case where α_1 has a (univariate) normal distribution with mean 0 and variance σ_α^2. Assume that the distribution of $y_1|\alpha_1$ is a fat-tailed distribution, which is a mixture of 0.95 normal distribution and 0.05 Cauchy distribution. Then,

$$\begin{aligned}\phi(y_1, \alpha_1) = &\log\left[0.95\exp\left(-0.5(y_1-\alpha_1)^2\Big/\sigma_y^2\right) + 0.05\sqrt{2/\pi}\Big/\left(1+(y-\alpha_1)^2/\sigma_y^2\right)\right] \\ &- 0.5\alpha_1^2/\sigma_\alpha^2 + \text{const}\end{aligned} \tag{9.7}$$

whereas if y_1 is assumed to have a normal distribution,

$$\phi(y_1, \alpha_1) = -0.5(y_1-\alpha_1)^2/\sigma_y^2 - 0.5\alpha_1^2/\sigma_\alpha^2 \ + \text{const} \tag{9.8}$$

where "const" denotes some constant independent of α_1. There are two drawbacks to the use of equation (9.8). If the value of y_1 is an outlier from the point of the normal model, then it will have too much influence on the mode of the estimate of $p(\alpha_1|y_1)$. Also, since the variance

$$\sigma_{\alpha_1|y_1}^2 = \left\{D_{\alpha_1\alpha_1}^2\phi(y_1, \beta_i)\right\}^{-1} = \left[1/\sigma_y^2 + 1/\sigma_\alpha^2\right]^{-1} \tag{9.9}$$

is independent of the value of y_1 observed, $\sigma_{\alpha_1|y_1}^2$ will be underestimated. This is incorrect behavior, since if y_1 is an outlier, it contains (almost) no information about the value of $p(\alpha_1|y_1)$. So, $p(\alpha_1|y_1)$ should be almost equal to $p(\alpha_1)$. The likelihood function based on equation (9.7) has the desired behavior.

To calculate expression (9.6), it is necessary to maximize $\phi(y_1, \alpha_1)$ with respect to α_1, and to calculate its Hessian matrix with respect to α_1.

For the maximization, we employ the Newton-Raphson algorithm. Let $\beta_0 = \mu_{\alpha_1}$

$$\beta_{i+1} = \beta_i - \left\{D_{\alpha_1\alpha_1}^2\phi(y_1, \beta_i)\right\}^{-1}\left(D_{\alpha_1}\phi(y_1, \beta_i)\right) \tag{9.10}$$

This operation is carried out a fixed number, r, times and then $\hat{\alpha}_1(y_1) \approx \beta_r$. For "well behaved" problems, the sequence β_i converges quadratically to $\hat{\alpha}_1(y_1)$. We approximate $p(\alpha_1|y_1)$ by a multivariate normal with

$$\begin{aligned}\mu_{\alpha_1|y_1} &= \beta_r \\ \sigma_{\alpha_1|y_1}^2 &= \left\{-D_{\alpha_1\alpha_1}^2\phi(y_1, \beta_r)\right\}^{-1}\end{aligned}$$

and approximate $p(\alpha_2|y_1)$ by a multivariate normal with

$$\begin{aligned}\mu_{\alpha_2|y_1} &= T(\beta_r, y_1)\\ \sigma^2_{\alpha_2|y_1} &= D_{\alpha_1} T_1(\beta_r, y_1)\sigma^2_{\alpha_1|y_1} D_{\alpha_1} T_1(\beta_r, y_1)' + \sigma^2_\eta\end{aligned}$$

Now,

$$p(y_2|y_1) = \int_{-\infty}^{\infty} p(y_2|\alpha_2)\, p(\alpha_2|y_1)\, \mathrm{d}\alpha_2 \tag{9.11}$$

As above, we maximize the integrand of equation (9.11) with respect to α_2 and use the Laplace approximation to the integral. This produces the sequence of conditional probabilities $p(y_i|y_{i-1})$. The log-likelihood function for the observed sequence y_i is given by

$$\sum_{i=1}^{n} \log\Big(p(y_i|y_{i-1})\Big) \tag{9.12}$$

9.1 Parameter estimation

Although we have not explicitly shown them, the conditional likelihood functions $p(y_i|y_{i-1})$ depend on a number of parameters. These parameters include the specification of T, other parameters in the probability density $p(y_i|\alpha_i)$, and parameters that determine σ^2_η. If we denote these parameters by θ and write $\big(p(y_i|y_{i-1}, \theta)\big)$ to indicate this dependence, the log-likelihood function becomes

$$\sum_{i=1}^{n} \log\Big(p(y_i|y_{i-1}, \theta)\Big) \tag{9.13}$$

The maximum likelihood estimates for the parameter vector θ are found by maximizing expression (9.13) with respect to θ.

9.2 The stochastic volatility model

The version of the stochastic volatility model presented here is from [2].

It is assumed that y_i has a multivariate normal distribution with $\mu_{y_i} = 0$ and covariance matrix $\Omega_i(\alpha_i) = H_i(\alpha_i) R H_i(\alpha_i)$. $H_i(\alpha_i)$ is an $m \times m$ diagonal matrix whose j^{th} element on the diagonal is given by $\exp(\alpha_{ij})/2$, where the α_{ij} satisfy the relationship

$$\alpha_i = w + \text{elem\_prod}(\delta, \alpha_{i-1}) + \text{elem\_prod}(\lambda_1, y_{i-1}) + \text{elem\_prod}(\lambda_2, |y_{i-1}|) + \eta_i \tag{9.14}$$

where, in turn, η_i is a multivariate normal random variable with $\mu_{\eta_i} = 0$ and $\sigma^2_{\eta_i} = \sigma^2_\eta$. If u and v are two vectors with j^{th} component u_j and v_j, elem_prod(i, v) is the vector with j^{th} component $u_j v_j$. R is an $m \times m$ positive definite matrix satisfying $r_{jj} = 1$, that is, a correlation matrix. Then,

$$\log\big(p(y_i|\alpha_i)\big) = -0.5 \log|\Omega_i(\alpha_i)| - 0.5 y_i'\, \Omega_i(\alpha_i)^{-1} y_i \tag{9.15}$$

and the distribution of $\alpha_i|y_{i-1}$ is multivariate normal, with mean vector and covariance matrix given by

$$\mu_{\alpha_i|y_{i-1}} = w + \text{elem\_prod}(\delta, \mu_{\alpha_{i-1}|y_{i-1}}) + \text{elem\_prod}(\lambda, y_{i-1}) \tag{9.16}$$

$$\sigma^2_{\alpha_i|y_{i-1}} = i\,\text{diag}(\delta)\sigma^2_{\alpha_{i-1}|y_{i-1}}\text{diag}(\delta) + \sigma^2_\eta \tag{9.17}$$

$\text{diag}(\delta)$ is the diagonal matrix whose diagonal is equal to the vector δ.

$$\log\left(p(y_i|\alpha_i)\,p(\alpha_i|y_{i-1})\right) = -0.5\log|\Omega_i(\alpha_i)| - 0.5y_i'\Omega_i(\alpha_i)^{-1}y_i - 0.5\log|\sigma^2_{\alpha_i|y_{i-1}}| \tag{9.18}$$

$$- 0.5(\alpha_i - \mu_{\alpha_i|y_{i-1}})'(\sigma^2_{\alpha_i|y_{i-1}})^{-1}(\alpha_i - \mu_{\alpha_i|y_{i-1}}) \tag{9.19}$$

To perform the Newton-Raphson calculations, it is necessary to calculate the first and second derivatives of expression (9.18) with respect to the parameter vector α. This is the most involved part of the calculations and will depend on the particular form of the model. In the present case, the calculations are simplified by the fact that Ω_i only depends on α through the diagonal matrix $H(\alpha_i)$.

The probability density function $p(\alpha_1)$ is assumed to be multivariate normal with $\mu_{\alpha_1} = \theta_0$ and $\sigma^2_{\alpha_1} = 0$.

9.3 The data

The data consist of the daily Mark/Dollar and Yen/dollar exchange rates and the U.S. and Japanese stock index data. There are 1301 time periods, with some missing data. The missing data, which are denoted by the impossibly large value of 10,000, were replaced with the average from the period before and after. They can, however, easily be estimated in the model, if desired.

9.4 The results

The model was fit with various combinations of the parameters, and the log-likelihood was examined to investigate the improvement in fit due to the addition of the parameters. See Table 9.1.

The parameters θ_0 and λ_2 did not produce a significant improvement to the fit. λ_2 measures the asymmetry in the response of the variance to positive and negative shocks.

Here are the parameter estimates and their standard deviations for the model with $w, \delta, R, \sigma^2_\eta$, and λ_1:

index	name	value	std.dev
1	w(1)	-1.3749e-001	4.9434e-002
2	w(2)	-6.5649e-001	1.6161e-001
3	w(3)	3.1693e-002	1.0574e-002
4	w(4)	-1.2973e-002	1.5375e-002

Parameters in model	Number of parameters	Log-likelihood
$w, \delta, R, \sigma_\eta^2$	24	3774.7
$w, \delta, R, \sigma_\eta^2, \lambda_1$	28	3806.6
$w, \delta, R, \sigma_\eta^2, \lambda_1, \theta_0$	32	3808.6
$w, \delta, R, \sigma_\eta^2, \lambda_1, \theta_0, \lambda_2$	36	3811.2

Table 9.1

```
 5  lambda1(1) 1.5564e-001 4.9688e-002
 6  lambda1(2) 1.8647e-001 6.9525e-002
 7  lambda1(3) -6.9265e-002 1.4158e-002
 8  lambda1(4) -1.6689e-001 3.1626e-002
 9  delta(1)   8.2229e-001 4.6074e-002
10  delta(1)   5.0848e-001 1.0785e-001
11  delta(1)   9.5763e-001 1.4602e-002
12  delta(1)   9.3610e-001 1.8812e-002
29  R(1,1)     1.0000e+000 0.0000e+000
30  R(1,2)     5.3821e-001 2.2883e-002
31  R(1,3)     -7.1704e-002 2.9477e-002
32  R(1,4)     -3.8796e-002 2.9278e-002
33  R(2,1)     5.3821e-001 2.2883e-002
34  R(2,2)     1.0000e+000 0.0000e+000
35  R(2,3)     -1.2932e-001 2.9111e-002
36  R(2,3)     -4.1466e-002 2.9468e-002
37  R(3,1)     -7.1704e-002 2.9477e-002
38  R(3,2)     -1.2932e-001 2.9111e-002
39  R(3,3)     1.0000e+000 0.0000e+000
40  R(1,4)     8.8811e-002 2.9085e-002
41  R(4,1)     -3.8796e-002 2.9278e-002
42  R(4,2)     -4.1466e-002 2.9468e-002
43  R(4,3)     8.8811e-002 2.9085e-002
44  R(4,4)     1.0000e+000 0.0000e+000
45  Omega(1,1) 6.5973e-001 6.3099e-002
46  Omega(1,2) 1.9827e-001 1.6129e-002
47  Omega(1,3) -1.3395e-001 5.4982e-002
```

```
  48   Omega(1,4) -3.5161e-002 2.6676e-002
  49   Omega(2,1) 1.9827e-001 1.6129e-002
  50   Omega(2,2) 2.0570e-001 2.3994e-002
  51   Omega(2,3) -1.3489e-001 3.2608e-002
  52   Omega(2,4) -2.0985e-002 1.5016e-002
  53   Omega(3,1) -1.3395e-001 5.4982e-002
  54   Omega(3,2) -1.3489e-001 3.2608e-002
  55   Omega(3,3) 5.2895e+000 5.7872e-001
  56   Omega(3,4) 2.2791e-001 7.9318e-002
  57   Omega(4,1) -3.5161e-002 2.6676e-002
  58   Omega(4,2) -2.0985e-002 1.5016e-002
  59   Omega(4,3) 2.2791e-001 7.9318e-002
  60   Omega(4,4) 1.2451e+000 1.7043e-001
  61   Z(1,1)     2.3967e-001 7.4268e-002
  62   Z(1,2)     2.0711e-001 5.5599e-002
  63   Z(1,3)     3.8832e-002 1.8505e-002
  64   Z(1,4)     2.4097e-002 2.0344e-002
  65   Z(2,1)     2.0711e-001 5.5599e-002
  66   Z(2,2)     4.6309e-001 1.1143e-001
  67   Z(2,3)     3.4298e-002 2.3017e-002
  68   Z(2,4)     9.6831e-003 2.9999e-002
  69   Z(3,1)     3.8832e-002 1.8505e-002
  70   Z(3,2)     3.4298e-002 2.3017e-002
  71   Z(3,3)     3.9101e-002 1.6885e-002
  72   Z(3,4)     2.4602e-002 1.1053e-002
  73   Z(4,1)     2.4097e-002 2.0344e-002
  74   Z(4,2)     9.6831e-003 2.9999e-002
  75   Z(4,3)     2.4602e-002 1.1053e-002
  76   Z(4,4)     9.6109e-002 3.4268e-002
```

The AD Model Builder TPL file for the model is given below:

```
DATA_SECTION
  init_int ndim
  init_int nobs
  int ndim1
  int ndim2
 !! ndim1=ndim*(ndim+1)/2;
 !! ndim2=ndim*(ndim-1)/2;
  init_matrix Y(1,nobs,1,ndim)
 LOC_CALCS
  // replace missing values (10000) with the average of before and after.
  for (int i=2;i<nobs;i++)
    for (int j=1;j<=ndim;j++)
```

```
      if (Y(i,j)==10000)
      {
        int i2=i+1;
        do
        {
          if (Y(i2,j)==10000)
            i2++;
          else
            break;
        }
        while(1);
        Y(i,j)=(Y(i-1,j)+Y(i2,j))/2.;
        if (Y(i,j)>100.0)   // did this work
          cerr << " Y(i,j) too big " << Y(i,j) << endl;
      }
 END_CALCS

PARAMETER_SECTION
  matrix h_mean(1,nobs,1,ndim)
  3darray h_var(1,nobs,1,ndim,1,ndim)
  number ldR;
  init_vector theta0(1,ndim,3);
  vector lmin(1,nobs)
  init_bounded_vector w(1,ndim,-10,10)
  vector w1(1,ndim)
  init_vector lambda(1,ndim,2)
  init_vector lambda2(1,ndim,-1)
  init_bounded_vector delta(1,ndim,0,.98)
  sdreport_matrix R(1,ndim,1,ndim)
  sdreport_matrix Omega(1,ndim,1,ndim)
  matrix ch_R(1,ndim,1,ndim)
  matrix Rinv(1,ndim,1,ndim)
  init_bounded_vector v_R(1,ndim2,-1.0,1.0)
  sdreport_matrix Z(1,ndim,1,ndim)
  matrix ch_Z(1,ndim,1,ndim)
  init_bounded_vector v_Z(1,ndim1,-1.0,1.0)
  matrix S(1,ndim,1,ndim);
  objective_function_value f
INITIALIZATION_SECTION
  delta 0.9
PROCEDURE_SECTION
```

```
  fill_the_matrices();
  int sgn;
  ldR=ln_det(R,sgn);
  Rinv=inv(R);
  dvar_vector tmp(1,ndim);
  dvar_matrix sh(1,ndim,1,ndim);
  h_mean(1)=theta0;
  h_var(1)=0;
  for (int i=2;i<=nobs;i++)
  {
    dvar_vector tmean=update_the_means(w,h_mean(i-1),Y(i-1));
    dvar_matrix v=update_the_variances(h_var(i-1));
    tmp=tmean;
    dvar_vector h(1,ndim);
    dvar_vector gr(1,ndim);
    for (int ii=1;ii<=4;ii++) // do the Newton-Raphson 4 times
    {
      xfp12(tmp, Y(i),tmean,v,gr,sh); // get 1st and 2nd derivatives
      h=-solve(sh,gr); //sh is hessian and gr is the gradient
      tmp+=h; // add new step h
    }
    double nh=norm2(value(h)); // check size of h for convergence
    if (nh>1.e-1)
      cout << "No convergence in NR " << nh << endl;
    if (nh>1.e+02)
    {
      f+=1.e+7;  // this ensures that the function minimizer will take a
      return;   // smaller step
    }
    h_mean(i)=tmp;
    h_var(i)=inv(sh);
    lmin(i)=fp(tmp,Y(i),tmean,v);
    int sgn;
    f+=lmin(i)+0.5*ln_det(sh,sgn); // Laplace approximation
  }
  f-=0.5*nobs*ndim*log(2.*PI);
  Omega=S;

FUNCTION dvar_vector update_the_means(dvar_vector& w,dvar_vector& m,dvector& e)
  dvar_vector tmp= w+elem_prod(delta,m)+elem_prod(lambda,e);
  if (active(lambda2))
    tmp+=elem_prod(lambda2,fabs(e));
```

```
  return tmp;

FUNCTION dvar_matrix update_the_variances(dvar_matrix& v)
  dvar_matrix tmp(1,ndim,1,ndim);
  for (int i=1;i<=ndim;i++)
  {
    for (int j=1;j<=i;j++)
    {
      tmp(i,j)=delta(i)*delta(j)*v(i,j);
      if (i!=j) tmp(j,i)=tmp(i,j);
    }
  }
  tmp+=Z;
  return tmp;

FUNCTION dvariable fp(dvar_vector& h, dvector& y, dvar_vector& m,dvar_matrix& v)
  dvar_vector eh=exp(.5*h);
  for (int i=1;i<=ndim;i++)
  {
    for (int j=1;j<=i;j++)
    {
      S(i,j)= eh(i)*eh(j)*R(i,j);
      if (i!=j) S(j,i)=S(i,j);
    }
  }

  dvariable lndet;
  dvariable sgn;
  dvar_vector u=solve(S,y,lndet,sgn);
  dvariable l;
  l=.5*lndet+.5*(y*u);
  dvar_vector hm=h-m;
  w1=solve(v,hm,lndet,sgn);
  l+=.5*lndet+.5*(w1*hm);
  return l;

FUNCTION void xfp12(dvar_vector& h, dvector& y,dvar_vector& m,dvar_matrix& v,
 dvar_vector gr,dvar_matrix& hess)
  dvar_vector ehinv=exp(-.5*h);
  dvariable lndet;
  dvariable sgn;
  dvar_vector ys=elem_prod(ehinv,y);
```

```
  dvar_vector u=Rinv*ys;
  gr=0.5;
  dvar_vector vv=elem_prod(ys,u);
  gr-=.5*vv;
  dvar_vector hm=h-m;
  dvar_vector w=solve(v,hm,lndet,sgn);
  gr+=w;
  for (int i=1;i<=ndim;i++)
  {
    for (int j=1;j<=i;j++)
    {
      hess(i,j)=0.25*ys(i)*ys(j)*Rinv(i,j);
      if (i!=j) hess(j,i)=hess(i,j);
    }
  }
  for (i=1;i<=ndim;i++)
  {
    hess(i,i)+=.25*vv(i);
  }
  hess+=inv(v);

FUNCTION fill_the_matrices
  int ii=1;
  ch_Z.initialize();
  for (int i=1;i<=ndim;i++)
  {
    for (int j=1;j<=i;j++)
      ch_Z(i,j)=v_Z(ii++);
    ch_Z(i,i)+=0.5;
  }
  Z=ch_Z*trans(ch_Z);
  ch_R.initialize();
  ii=1;
  for (i=1;i<=ndim;i++)
  {
    for (int j=1;j<i;j++)
      ch_R(i,j)=v_R(ii++);
    ch_R(i,i)+=0.1;
    ch_R(i)/=norm(ch_R(i));
  }
  R=ch_R*trans(ch_R);
```

```
REPORT_SECTION
  report<<"observed"<<Y<<endl;
  for (int i=1;i<=nobs;i++)
  {
    report<< "mean" <<endl;
    report<< h_mean(i) <<endl;
    report<< "covariance" <<endl;
    report<<h_var(i)<<endl;
    report<<endl;
  }
  report<< "S(nobs) " << endl;
  report<< Omega << endl;
  report<< "Z " << endl;
  report<< Z << endl;
  report<< "R " << endl;
  report<< R << endl;

TOP_OF_MAIN_SECTION
  arrmblsize=20000000;
  gradient_structure::set_CMPDIF_BUFFER_SIZE(25000000);
  gradient_structure::set_GRADSTACK_BUFFER_SIZE(1000000);
```

Chapter 10

Using Vectors of Initial Parameter Types

This chapter introduces three new AD Model Builder types. They are

```
init_number_vector
init_vector_vector
init_matrix_vector
```

plus the bounded versions of these

```
init_bounded_number_vector
init_bounded_vector_vector
init_bounded_matrix_vector
```

To understand the usefulness of these objects, consider an application that has two `init_number` objects:

```
PARAMETER_SECTION
  init_bounded_number a1(0.2,1.0,1)
  init_bounded_number a2(-1.0,0.3,2)
```

This creates two bounded numbers with different upper and lower bounds becoming active in different phases of the minimization. Now, however, suppose that the number of numbers we wish to have in the model depends on some integer read in at run time, such as:

```
DATA_SECTION
  init_int n
 //  ...

PARAMETER_SECTION
  // want to have n numbers
  init_bounded_number a1(0.2,1.0,1)
  init_bounded_number a2(-1.0,0.3,2)
  // ....
  init_bounded_number an(-4.0,-3.0,n)
```

The above code is a sketch of what we want to achieve. It cannot be accomplished with that kind of coding, of course, because at compile time, we don't have the value for n, and in any event, if n is large, this sort of coding is boring. Dynamic arrays are the answer to this problem. One could try the following:

```
DATA_SECTION
  init_int n
 //  ...

PARAMETER_SECTION
  // want to have n numbers
  init_bounded_vector a(1,n,-1.0,1.0,1)
```

but this won't work, because for an `init_bounded_vector`, the bounds and the starting phase are the same for all components of the vector. The `init_bounded_number_vector` class is intended to solve this problem.

```
DATA_SECTION
  init_int n
 //  ...

PARAMETER_SECTION
  // need to create some vectors to hold the bounds and
  // phase numbers
 LOC_CALCS
  dvector lb(1,n);
  dvector ub(1,n);
  ivector ph(1,n);
  // get the desired values into lb,ub,ph somehow
  lb.fill_seqadd(1,0.5);
  ub.fill_seqadd(2,0.5);
  ph.fill_seqadd(1,1);
 END_CALCS
  init_bounded_number_vector a(1,n,lb,ub,ph)
```

Then `a(1)` is an object of type `init_bounded_number` with bounds `lb(1)` and `ub(1)` becoming active in phase `ph(1)`. Any of these three fields can be replaced with a number or integer if the bound or phase number is constant, such as

```
  init_bounded_number_vector a(1,n,1.0,ub,2)
```

where the lower bound is `1.0` and the phase number is `2`.

Chapter 11

Creating Dynamic Link Libraries with AD Model Builder

For performance reasons, many nonlinear modeling routines for packages such as Splus or Gauss, or spreadsheets such as Excel, are written in other languages, such as C or FORTRAN, and compiled as DLLs or shared libraries. Due to AD Model Builder's support for nonlinear statistical modeling, it is generally much faster and easier to produce the code for a nonlinear statistical model with ADMB rather than C or FORTRAN. This code can then be put into a shared library (DLL) and called from Splus as though it were a part of the language.

This section focuses on creating DLLs for Splus Version 4 Release 3, Gauss under Windows 95/NT, or for the R programming environment under Windows 95/NT or Linux. The construction can be easily modified to produce DLLs, which can be used by other programs, such as Visual Basic, or spreadsheets like Excel.

There are two example programs: a very simple example to illustrate the ideas, and a program to estimate the parameters from a mixture of two bivariate normal distributions.

We begin with the simple example. We wish to minimize the function f given by

$$f = (x_1 - 1.0)^2 + \sum_{i=1}^{n-1} (x_{i+1} - x_i)^2$$

with respect to the n-dimensional vector x. The starting values are $x = (0, 0, \ldots, 0)$.

While this is a quadratic function that can be solved by special methods, we do not use this special structure, because we want to illustrate the technique on general nonlinear models.

There are three modifications to a stand-alone AD Model Builder program that must be made to produce a DLL.

1. The command line option `-dll` is given to the `tpl2cpp` program, which translates the template file into a C++ file. For Gauss, replace the `-dll` option with the `-gausdll` option.

2. The user must decide what data and parameter objects are to be passed to, or returned from, the DLL, and modify the TPL file accordingly.

3. The interface code must be written in the calling language.

Objects that are to be passed into, or returned from, the DLL are identified by putting the prefix `dll_` before their declarations.

In this example, the number of independent variables is passed from the calling program to the DLL. Thus, `init_int nvar` is modified to `dll_init_int nvar`. The calling program expects to get the minimum value `freturn` and the minimizing values of the init_vector x returned to it, so they are declared to be of type `dll_number` and `dll_init_vector`.

```
DATA_SECTION
  dll_int nvar
PARAMETER_SECTION
  dll_init_vector x(1,nvar)
  dll_number freturn
  objective_function_value f
PROCEDURE_SECTION
  f=square(x(1)-1.0);
  for (int i=1;i<nvar;i++)
  {
    f+=square(x(i+1)-x(i));
  }
  freturn=f;
```

11.1 Compiling the code to produce a DLL

The exact form of the commands used to produce a DLL, or shared library, depend on the compiler used and the operating system.

Assuming that the template file is named `xxxx.tpl|` for NT/9?, then using the gcc2.95-mingw32 compiler, the commands are

```
tpl2cpp -dll %1

 C++ -fpermissive -O3 -c -DBUILDING_DLL=1 -D__GNUDOS__ -I. i
  -If:/admodel/include -o %1.o %1.cpp

dllwrap -def %1.def --implib lib%1.a --driver-name \cplus\ -o %1.dll %1.o
   -Lf:/admodel/lib -ladmod -ladt -lado -lm
```

where the symbol `%1` (this is a batch file argument, which would be `$1` for Linux) should be replaced by `xxxx`.

Of course, you don't want to type all this every time, so the commands should be replaced in a `.bat` file, such as `makedll.bat`. Then, to compile the TPL into a DLL, it is only necessary to type

```
makeadll xxxx
```

where `xxxx.tpl` is the template file. For debugging purposes, you may find that you want to edit the `.cpp` file, so you will not want to run `tpl2cpp` every time. In that case, the first line should be removed from the `.bat` file.

To call the DLL from Splus, the `dll.load` function is used to load the library.

```
dll.load("simpdll.dll",symbol="simpdll")
n<-100
x<-rep(0,n)
freturn<-0
ans<-.C("simpdll",as.integer(n),x = as.double(x),as.double(f)," -sp -crit 1.e-8 -nohess")
```

The final parameter, `-sp -crit 1.e-8 -nohess`, is a string that serves the same function as command line options in AD Model Builder programs. The `-sp` option tells the DLL that it is being run from Splus, so it can print into the Splus command window. The `-crit` option sets the convergence criterion for the magnitude of the components of the gradient, and the `-nohess` option suppresses the calculation of the Hessian at the minimum. It must be present, although it can be blank.

It is necessary for Splus to find the DLL. If it has trouble doing so, a full path name can be used as in:

```
dll.load("c://mydlls//simpdll.dll",symbol="simpdll")
```

11.2 The Splus objects

At present, the objects for communication with Splus that can be put in the `DATA_SECTION` of the TPL file are

```
dll_init_int
dll_iinit_number
dll_iinit_vector
dll_init_matrix
dll_int
dll_number
dll_vector
dll_matrix
```

while in the `PARAMETER_SECTION`, they are

```
dll_init_number
dll_init_bounded_number
dll_init_vector
dll_init_bounded_vector
```

```
dll_init_matrix
dll_number
dll_vector
dll_matrix
```

These objects act the same as the corresponding AD Model Builder objects without the `dll_` prefix. For initial parameters, the difference is that they are assumed to get their initial values from Splus.

Note that by default, Splus stores elements of a matrix by columns, that is, contiguous areas of memory run down the columns. AD Model Builder stores its elements by rows, so that when a matrix objects is passed to it from Splus, it expects the object to be stored by column and does a transpose operation on it. At the conclusion of the AD Model Builder program, the object is passed back to Splus via the inverse operation. This process should be transparent to the user.

Gauss, on the other hand, stores a matrix by rows. In addition, Gauss passes a string as a `char *` rather than the `char **` employed by Splus. Using the `-gaussdll` option ensures that Gauss matrices and strings will be handled properly.

11.3 Debugging the DLLs

Before you compile your program as a DLL, it is easiest if you first compile it as a stand-alone application and debug it. Then you can simply put the `dll_` prefix before those objects you wish to have passed to and from the calling program. Also is inconvenient to debug the DLLs from Splus directly. Errors in the code usually cause Splus to crash. Also, printing results to the screen from a DLL can be problematic if the calling program does not provide for it. To alleviate this problem, it is possible to call the function in the DLL from a C or C++ routine. This enables the use of symbolic debuggers, etc., to debug the code, and enables screen I/O. Here is C code that can load the DLL and call the function:

```
#include <stdio.h>
#include <windows.h>

typedef __declspec(dllexport) void _export (*MYPROC)(int *_nvar,
  double *_x,
  double *_freturn,
  char ** sp_options);

VOID main(int argc,char * argv[])
{
  HINSTANCE h;
  MYPROC p;
  /* Now invent the objects we need to pass to the DLL */
  int nvar=50;
```

```
  double x[50];
  double freturn;
  char * str;
  int i;
  char * str = " -nox -crit 1.e-7 ";
  h=LoadLibrary("simpdll"); /* load the DLL */
  if (h)
  {
    printf("loaded simdll.dll successfully\n");
    /* get pointer to the function */
    p=(MYPROC) GetProcAddress(h,"_simpdll");
    if (p)
    {
      freturn=0.0;
      for (i=0;i<nvar;i++)
        x[i]=0.0;
      p(&nvar,x,&freturn,&str);

      printf("function value = %lf\n",&freturn);
      for (i=0;i<nvar;i++)
        printf("x[%d]= %lf\n",i,x[i]);

    }
    else
      printf("Can't find function simdll in DLL\n");
  }
  else
   printf("Can't load simdll.dll\n");
}
```

This code can be compiled with the command

```
gcc -otestsim.exe testsim.c
```

which will produce the program `testsim.exe`. Running this program will load the DLL, find the function in it, and call it. At the end, it will report the results obtained.

11.4 Understanding what is being passed to the DLL

The most difficult part of calling a C++ DLL from some other type of application is understanding the correct formalism for passing different objects between the two. For example, a string in Visual Basic may be a very different object from the simple `char *` (pointer to char) of the C and C++ languages. If you get it wrong, then the program will usually crash when the code in the DLL tries to access the object. The easiest way to debug this is to have

the DLL code print out the values of the passed objects. (However, keep in mind that simply trying to access the values for printing may cause the program to crash.)

Consider the C++ for the example TPL code given above:

```
#include <admodel.h>

#include <simpdll.htp>

model_data::model_data(splus_args& ad_spa)
{
  nvar.allocate(ad_spa.nvar,"nvar");
}

model_parameters::model_parameters(int sz,
  int argc,
  char * argv[],
  splus_args& ad_spa) :
 ad_comm(argc,argv), model_data(ad_spa) , function_minimizer(sz)
{
  initializationfunction();
  x.allocate(ad_spa.x,1,nvar,"x");
  freturn.allocate(ad_spa.freturn,"freturn");
  f.allocate("f");
}

void model_parameters::userfunction(void)
{
  f=square(x(1)-1.0);
  for (int i=1;i<nvar;i++)
  {
    f+=square(x(i+1)-x(i));
  }
  freturn=f;
}

void model_parameters::preliminary_calculations(void){}

model_data::~model_data()
{}

model_parameters::~model_parameters()
{}
```

```
void model_parameters::report(void){}

void model_parameters::final_calcs(void){}

void model_parameters::set_runtime(void){}

#ifdef _BORLANDC_
  extern unsigned _stklen=10000U;
#endif


#ifdef __ZTC__
  extern unsigned int _stack=10000U;
#endif

  long int arrmblsize=0;
extern "C" {

#if !defined(__delcspec)
#  define __declspec(x)
#endif

#if !defined(__BORLANDC__)
#  define _export
#endif

__declspec(dllexport) void _export simpdll(int *_nvar,
  double *_x,
  double *_freturn,
  char ** sp_options)
{
  int argc=1;
  try {
    char **argv=parse_sp_options("simpdll",argc,*sp_options);
    do_dll_housekeeping(argc,argv);
    splus_args ad_spa(_nvar,_x,_freturn);
    gradient_structure::set_NO_DERIVATIVES();
    gradient_structure::set_YES_SAVE_VARIABLES_VALUES();
  #if defined(__GNUDOS__) || defined(DOS386) || defined(__DPMI32__) || \
     defined(__MSVC32__)
      if (!arrmblsize) arrmblsize=150000;
  #else
```

```
    if (!arrmblsize) arrmblsize=25000;
  #endif
    model_parameters mp(arrmblsize,argc,argv,ad_spa);
    mp.iprint=10;
    mp.preliminary_calculations();
    mp.computations(argc,argv);
    cleanup_argv(argc,&argv);
    ad_make_code_reentrant();
  }
  catch (spdll_exception spe){
    if (ad_printf && spe.e) (*ad_printf) ("abnormal exit from newtest\n");
  }
}
}
```

For now, we are only interested in the part of the code after the beginning of the function

```
__declspec(dllexport) void _export simpdll(int *_nvar,
  double *_x,
  double *_freturn,
  char ** sp_options)
{
  int argc=1;
  try {
  .....
```

Modify this code to:

```
__declspec(dllexport) void _export simpdll(int *_nvar,
  double *_x,
  double *_freturn,
  char ** sp_options)
{
  cout << " nvar = " << *_nvar << endl;
  return;
  int argc=1;
  try {
   .....
```

If everything is OK, this will simply print out the value of `nvar` and return to the calling program. Then the value of `x` can be printed out as well, with code like:

```
__declspec(dllexport) void _export simpdll(int *_nvar,
  double *_x,
  double *_freturn,
  char ** sp_options)
```

```
{
  cout << " nvar = " << *_nvar << endl;
  cout << " x = " << endl;
  for (int i=0;i<*_nvar;i++)
    cout << _x[i] << endl;
  cout << " freturn = " << *_freturn << endl;
  cout << " sp_options = " << *sp_options << endl;
  return;
  int argc=1;
  try {
   .....
```

If you don't have access to the screen, the above code can be modified to print to a file.

```
__declspec(dllexport) void _export simpdll(int *_nvar,
  double *_x,
  double *_freturn,
  char ** sp_options)
{
  ofstream ofs("logfile");
  ofs << " nvar = " << *_nvar << endl;
  ofs << " x = " << endl;
  for (int i=0;i<*_nvar;i++)
    ofs << _x[i] << endl;
  ofs << " freturn = " << *_freturn << endl;
  ofs << " sp_options = " << *sp_options << endl;
  return;
  int argc=1;
  try {
   .....
```

After running the program, you should find the values of the objects printed into a file named `logfile`.

Splus passes objects to the DLL by address, that is, it finds the address in memory of the object and passes that value. So the integer `nvar` is not passed itself, but the address is. In C or C++, you get the address of an object with the `&` operator. Given the address of an object, you access the object with the `*` operator. In the above code, `_nvar` is the address of an integer passed by the calling program to the DLL and `*_nvar` accesses the object. So, the line of code

```
*_nvar=5;
```

will set the values of the integer to 5 back in the calling program. When Splus passes a vector object, it passes the address of the first element in the vector. So, if the vector is a vector of double precision numbers (an object of type `double` in C), it will pass a pointer to

`double`. So in the above code, `_x` is the address of the first element of the vector and `*_x` is the first element, so

```
*_x=12.55;
```

will set the first element in the vector equal to `12.55`. To access other elements of the vector, use the `[]` operators.

```
x[0]=12.55; // same as *_x=12.55
x[4]=-2.5; // sets the 5 element equal to -2.5
```

11.5 Passing strings from Splus to a DLL

A string in C is a pointer to an array of elements of type `char`. It might be logical to conclude that Splus would pass the address of the first element of the array. This is not the case. Splus passes the address of the object pointing to the first element of the array (a `char **` in C). So in the above code, if you want to print the second element of the string, point `sp_options` to the standard output device:

```
cout << (*sp_options)[1] << endl; // print the second element of the string
```

You must use the parentheses, because the `[]` operation has higher precedence than does the `*` operation.

11.6 A mixture of two bivariate normal distributions

This is a more complicated example. Let x_i be a collection of 2-dimensional vectors drawn at random from a mixture of two bivariate normal distributions with means μ_i and covariance matrices Σ_i. The data to be analyzed are shown here. They consist of 500 points from the mixture, with 25% in one component and 75% in the other component. Both samples have positively correlated components, so they both lie near the line $y = x$. This makes them difficult to separate. The means used for the simulations were

```
(0,0)    (1,0)
```

while the covariance matrices used for the simulation were

```
1.77778 4.74074   1.77778 2.37037
4.74074 14.4198   2.37037 4.93827
```

The estimates for these parameters obtained by the model were

```
(0.026,0.059) (1.266,0.287)

1.42409 3.86336  1.66321 2.34985
3.86336 12.2286  2.34985 4.94363
```

The estimated proportions were

```
0.343  0.657
```

See Figure 11.1.

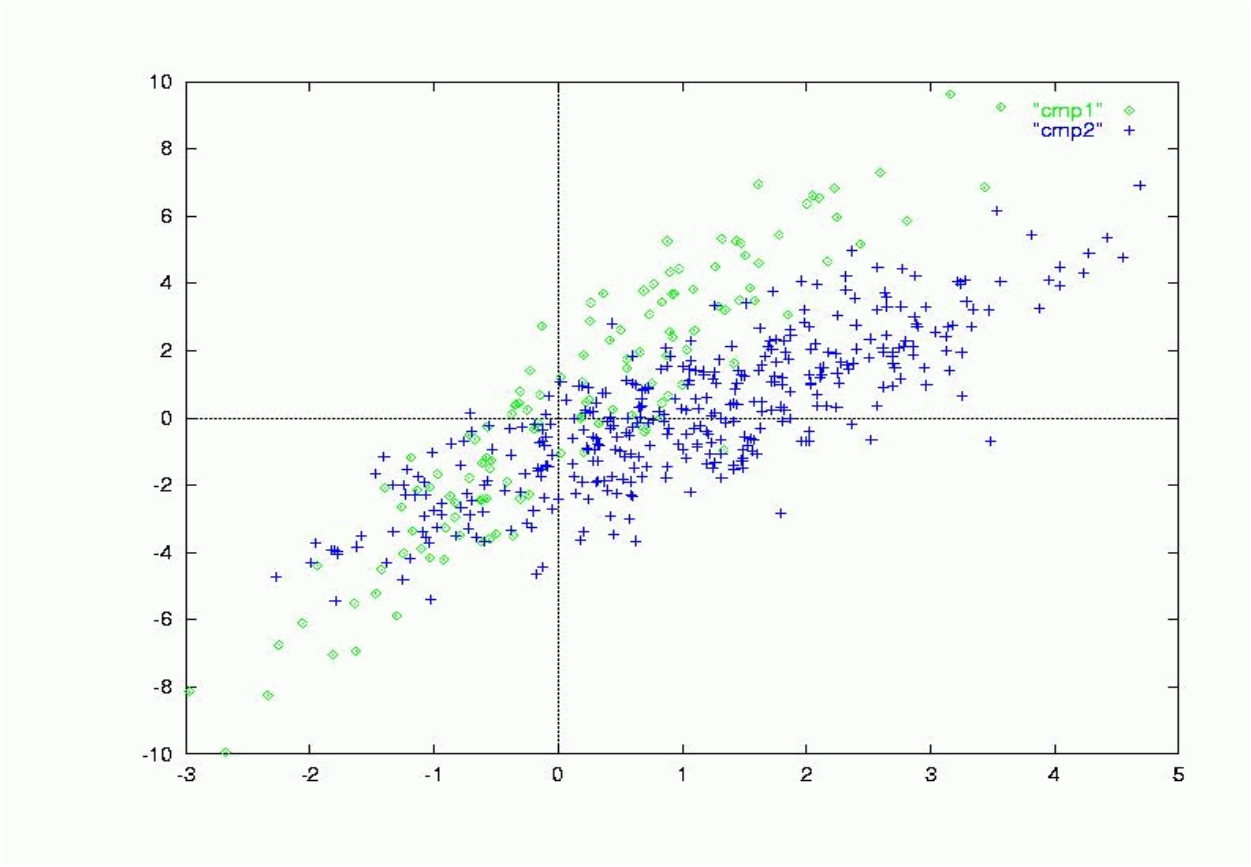

Figure 11.1

The minimization is carried out in three phases. For the first phase, only the proportions of the mixture are estimated, with the parameters that determine the covariance matrices and the means held fixed. For the second phase, the covariance matrices are estimated as well, with the means held fixed. For the third and final phase, all the parameters are estimated. The idea is that the user should start with some good estimates for the means. Of course, the model could be run several times with different initial estimates and if different solutions are obtained, then the one with the best fit would be chosen.

The initial values used for the means and standard deviations were

```
(-1,0)   (2,0)

1  0     1  0
0  1     0  1
```

The initial values used for the proportions were

```
0.5     0.5
```

The log-likelihood function for the sample is

$$\sum_{i=1}^{n} \log \Big\{ p_1 |\Sigma_1|^{-1/2} \exp\big(-0.5(x_i-\mu_1)' \Sigma_1^{-1}(x_i-\mu_1)\big) + p_2 |\Sigma_2|^{-1/2} \exp\big(-0.5(x_i-\mu_2)' \Sigma_2^{-1}(x_i-\mu_2)\big) \Big\} \tag{11.1}$$

The main technical difficulty in maximizing the log-likelihood function is parameterizing the covariance matrices in such a way that they will be positive definite. This is done by employing a "positivized" Choleksi decomposition. Σ_i as $\Sigma_i = C_i C_i' + \lambda I$, where C_i is a lower triangular matrix, $\lambda > 0$ is a "small" positive number, and I is the identity matrix. The proportions in the mixture are parameterized by a bounded vector of parameters that is normalized so that the components will sum to 1. The code for the example follows:

```
DATA_SECTION
  dll_int nobs
  dll_matrix obs(1,nobs,1,2)
PARAMETER_SECTION
  dll_init_bounded_vector pcoff(1,2,.02,1.1);
  dll_init_bounded_vector C1(1,3,-10.0,10.0,2)
  dll_init_bounded_vector C2(1,3,-10.0,10.0,2)
  dll_init_vector mu1(1,2,3)
  dll_init_vector mu2(1,2,3)
  dll_matrix S1(1,2,1,2)
  dll_matrix S2(1,2,1,2)
  dll_vector p(1,2)
  objective_function_value f
PROCEDURE_SECTION
  dvariable psum=sum(pcoff);
  f+=100.*square(log(psum+1.e-20));
  p=pcoff/(psum+1.e-20); // so p's satisfy constraints
  dvar_matrix tmp1(1,2,1,2);
  dvar_matrix tmp2(1,2,1,2);
  tmp1.initialize();
  tmp2.initialize();
  int ii=1;
  int i=0;
  for (i=1;i<=2;i++) { // fill lower triangle
    for (int j=1;j<=i;j++) {
      tmp1(i,j)=C1(ii);
      tmp2(i,j)=C2(ii);
      ii++;
```

```
    }
  }
  S1=tmp1*trans(tmp1); // form S1 S2 from Choleski decomp.
  S2=tmp2*trans(tmp2);
  for (i=1;i<=2;i++) { // to make positive definite
    S1(i,i)+=0.1;
    S2(i,i)+=0.1;
  }
  dvariable det1=sqrt(det(S1));
  dvariable det2=sqrt(det(S2));
  dvar_matrix S1inv=inv(S1);
  dvar_matrix S2inv=inv(S2);
  for (i=1;i<=nobs;i++) // add up minus log-likelihood
  {
    // add the 1.e-10 to avoid log(0) and for robustness
    f-= log(1.e-10+p(1)/det1*exp(-.5*(obs(i)-mu1)*S1inv*(obs(i)-mu1))
       +p(2)/det2*exp(-.5*(obs(i)-mu2)*S2inv*(obs(i)-mu2)));
  }
RUNTIME_SECTION
  maximum_function_evaluations 50,100,10000
REPORT_SECTION
  report << "First mean = " << endl << mu1 << endl;
  report << "First covariance matrix = " << endl<< S1 << endl;
  report << "Second mean = " << endl << mu2 << endl;
  report << "Second covariance matrix = " << endl << S2 << endl;
```

This example can be run by using the following Splus source code:

```
nobs<-scan("bimix.dat",n=1)
x<-matrix(scan("bimix.dat",skip=1),nrow=nobs,ncol=2,byrow=TRUE)
pcoff<-rep(.5,2)
C1<-rep(1,3)
C2<-rep(1,3)
C1[2]<-0
C2[2]<-0
p<-rep(0,2)
mu1<-rep(0,2)
mu1[1]<--1
mu2<-rep(0,2)
mu2[1]<-2
S1<-matrix(0,nrow=2,ncol=2)
S2<-matrix(0,nrow=2,ncol=2)
dll.load("bimix.dll",symbol="bimix")
ans<-.C("bimix",nobs=as.integer(nobs),as.double(x),pcoff=as.double(pcoff),
```

```
  C1=as.double(C1),C2=as.double(C2),mu1=as.double(mu1),mu2=as.double(mu2),
  S1=as.double(S1),S2=as.double(S2),p=as.double(p)," -sp -nohess ")
dll.unload("bimix.dll")
S1<-matrix(ans\$S1,nrow=2)
S2<-matrix(ans\$S2,nrow=2)
mu1<-ans\$mu1
mu2<-ans\$mu2
p<-ans\$p
print ("Estimated proportions")
print(p)
print ("Estimated mean for component 1")
print(mu1)
print ("Estimated mean for component 2")
print(mu2)
print ("Estimated covariance matrix for component 1")
print(S1)
print ("Estimated covariance matrix for component 2")
print(S2)
```

This code only works under NT/95 for Version 4 Release 3. Assuming that you have put the code where Splus can find it, you can run the example from Splus by typing

```
source("bimix.spl")
```

There is also a file, `bimix.r`, which will run the program under R. However, at present for Windows, the R version will not print out any intermediate results. So, be patient and the final estimates will appear when the minimization has converged. After the program executes, the parameter estimates can be found in the Splus variables `p`, `mu1`, `mu2`, `S1`, and `S2`.

11.7 Interpretation of the parameter estimates

If the user desires, they can remove the `-nohess` option and have the program compute estimates of the variances of the parameter estimates.

```
index  name   value     std.dev
   1   pcoff  3.5511e-01 1.5693e+00
   2   pcoff  6.7911e-01 2.9777e+00
   3   C1     1.1507e+00 7.9990e-02
   4   C1     3.3574e+00 2.8240e-01
   5   C1     9.2537e-01 1.7504e-01
   6   C2     1.2503e+00 7.7426e-02
   7   C2     1.8795e+00 1.2641e-01
   8   C2     1.1451e+00 8.3415e-02
```

```
 9   mu     2.6366e-02 1.2791e-01
10   mu     5.9418e-02 3.4832e-01
11   mu     1.2627e+00 1.4717e-01
12   mu     2.8665e-01 1.7818e-01
13   p      3.4336e-01 6.7238e-02
14   p      6.5664e-01 6.7238e-02
```

The program also reports the correlation matrix

```
index   name    value     std.dev     1     2      3      4      5      6      7      8      9     10     11     12     13     14
    1   pcoff  3.551e-01 1.569e+00  1.000
    2   pcoff  6.791e-01 2.977e+00  0.997  1.000
    3   C1     1.150e+00 7.999e-02 -0.039 -0.021  1.000
    4   C1     3.357e+00 2.824e-01 -0.094 -0.052  0.736  1.000
    5   C1     9.253e-01 1.750e-01  0.067  0.036  0.031 -0.394  1.000
    6   C2     1.250e+00 7.742e-02 -0.071 -0.039  0.156  0.266 -0.070  1.000
    7   C2     1.879e+00 1.264e-01 -0.016 -0.009 -0.066 -0.046 -0.087  0.613  1.000
    8   C2     1.145e+00 8.341e-02 -0.072 -0.039  0.031  0.343 -0.308  0.138 -0.116  1.000
    9   mu     2.636e-02 1.279e-01 -0.000 -0.000  0.147 -0.054  0.285  0.349  0.163 -0.212  1.000
   10   mu     5.941e-02 3.483e-01 -0.045 -0.024  0.198  0.160 -0.012  0.411  0.245 -0.066  0.861  1.000
   11   mu     1.262e+00 1.471e-01  0.115  0.063 -0.295 -0.521  0.257 -0.572 -0.170 -0.322 -0.225 -0.421  1.000
   12   mu     2.866e-01 1.781e-01  0.063  0.034 -0.237 -0.247  0.071 -0.482 -0.265  0.003 -0.363 -0.460  0.803  1.000
   13   p      3.433e-01 6.723e-02  0.148  0.081 -0.266 -0.636  0.450 -0.482 -0.111 -0.487 -0.001 -0.302  0.773  0.426  1.000
   14   p      6.566e-01 6.723e-02 -0.148 -0.081  0.266  0.636 -0.450  0.482  0.111  0.487  0.001  0.302 -0.773 -0.426 -1.000  1.000
```

Chapter 12

Command Line Options

AD Model Builder has a number of options that can be invoked at the command line. A list of current options can be displayed by typing the name of the application followed by `-?`.

You will see a display like:

```
AD Model Builder Copyright (c) 2008 Regents of the University of California
USAGE--kalman options
where an option consists of -option_tag followed by arguments if necessary
-ainp NAME      change default ascii input parameter file name to NAME
-binp NAME      change default binary input parameter file name to NAME
-est            only do the parameter estimation
-ind NAME       change default input data file name to NAME
-lmn N          use limited memory quasi newton -- keep N steps
-lprof          perform profile likelihood calculations
-prsave         save the independent variables from the profile calculations
-maxph N        increase the maximum phase number to N
-mcdiag         use diagonal covariance matrix for mcmc with diagonal values 1
-mcmc [N]       perform markov chain monte carlo with N simulations
-mcmult N       multiplier N for mcmc default
-mcr            resume previous mcmc
-mcrb N         modify the covariance matrix to reduce extremely high correlation
-mcnoscale      don't rescale step size for mcmc depending on acceptance rate
-mcprobe N      use probing strategy for mcmc with factor N
-mcseed N       seed for random number generator for markov chain monte carlo
-mccale N       rescale step size for first N evaluations
-mcsave N       save the parameters for every N'th simulation
-mceval         Go through the saved mcmc values from a previous mcsave
-mcpin NAME      Read the starting values for MCMC from the file NAME
-crit N         set gradient magnitude convergence criterion to N
-iprint N       print out function minimizer report every N iterations
-maxfn N        set maximum number of function eval's to N
-rs             if function minimizer can't make progress rescale and try again
-nox            don't show vector and gradient values in function minimizer screen
```

```
                report
-phase N        start minimization in phase N
-simplex        use simplex algorithm for minimization (new test version)
-sdonly         do delta method for std dev estimates without redoing hessian
-ams N          set arrmblsize to n (ARRAY_MEMBLOCK_SIZE)
-cbs N          set CMPDIF_BUFFER_SIZE TO N
-mno N          set the maximum number of independent variables to N
-gbs N          set GRADSTACK_BUFFER_SIZE TO N
-mdl N          set the maximum number of dvariables to N
-? or -help     this message
```

The version of AD Model Builder is printed. This can be useful to determine the version with which the application was compiled.

`-aind NAME`
By default, the program named `xxxx(.exe)` tries to read in its data from the file `xxxx.dat`. This option changes the data file to `NAME`.

`-ainp NAME`
This option changes to NAME the file from which the initial parameter estimates are read. The program expects the parameters to be in ASCII format, with comment lines beginning with `#`.

When a program is running, it produces parameter estimates in ASCII format, in files named `xxxx.p01`,..., `xxxx.par`. These files are in the proper format to be input back into the model and permit restarts at any phase of the minimization.

`-binp NAME`
This option changes to NAME the file from which the initial parameter estimates are read. The program expects the parameters to be in binary format.

When a program is running, it produces parameter estimates in binary format in files named `xxxx.b01`,..., `xxxx.bar`. These files are in the proper format to be input back into the model and permit restarts at any phase of the minimization.

Both ASCII and binary forms of the parameter files are supplied, because they have different advantages and disadvantages. ASCII files can be easily examined and edited. Binary files supply parameter values to the limit of machine precision in a compact format.

`-lmn N`
The limited memory Newton minimization option reduces the amount of memory necessary for holding the approximate Hessian inverse. It is of use particularly in problems with a large number of parameters (typically, > 1000). For many problems, it is not as efficient per function evaluation as is the default quasi-Newton method, although this is not always the case. `N` is the number of pass steps of information kept for the quasi-Newton update. Typically, a value in the range 5–20 is good.

`-lprof`

This option turns on the profile likelihood calculations. A variable for which profile likelihood calculations are performed must have been declared with the `likeprof_number` in the TPL file.

`-prsave`
This option causes the values of the independent variables for the profile likelihood points to be saved in a file named `xxx.pvl`, where `xxx` is the name of the variable being profiled. These values can be used later for starting the MCMC analysis at different values, which is useful for testing the mixing of the chain with respect to that parameter.

`-maxph N`
You may want to add extra phases to the minimization—usually because the standard set of phases has not converged. This will set the number of phases to `N`.

`-mcmc [N]`
This option turns on the the calculation of the Markov chain Monte Carlo routine. By default, the model will recalculate the approximate Hessian, so you may want to use the `-nohess` option if you don't wish to recalculate the Hessian. It is your responsibility to ensure that the Hessian data in the current directory are current. The `mcmc` routine will perform `N` simulations.

`-mcr`
Restart (and continue) a previous Markov chain Monte Carlo routine. This will continue from where the previous routine left off.

`-mcrb N`
See discussion of this option elsewhere in the manual.

`-mcsave N`
For the usual MCMC routine, the results from consecutive steps of the simulation are highly correlated. If the parameters of interest are expensive to compute, it may be advantageous to only compute every N^{th} one. This option saves the results so that they can be used in subsequent calculations.

`-mceval N`
This option will use the previously saved results from `mcmc` to evaluate parameters of interest. The function `mceval_phase()` can be useful here to only calculate the parameters during this phase.

`-nox`
This option suppresses the printing of the current `x` vector being sampled by the function minimizer. Printing this out can be a significant overhead for models with a large number of parameters. Also, it simply irritates some users.

`-ams N` `set arrmblsize to n (ARRAY_MEMBLOCK_SIZE)`

This option has the same effect as setting `arrmblsize` in the program code, but has the advantage that it can be done at runtime.

`-cbs N` `set CMPDIF_BUFFER_SIZE to n`
This option has the same effect as the `gradient_structure::set_CMPDIF_BUFFER_SIZE` function in the program code, but has the advantage that it can be done at runtime.

`-gbs N` `set GRADSTACK_BUFFER_SIZE`
This option has the same effect as the `gradient_structure::set_GRADSTACK_BUFFER_SIZE` function in the program code, but has the advantage that it can be done at runtime. *Also note that the size is in bytes here, whereas for the included code, it is in chunks of about 36 bytes.*

Chapter 13

Writing Adjoint Code

13.1 The necessity for adjoint code

When you write code for variable objects in AD Model Builder, all the derivatives are calculated for you in a transparent manner. To accomplish this, AD Model Builder must save certain information for later use. We shall refer to this as derivative information. Each arithmetic operation generates about 32 bytes of derivative information. If you have some simple function that has 20 arithmetic operations, it will therefore generate 640 bytes of derivative information every time it is called. The purpose of writing adjoint code is to reduce the amount of derivative information that must be calculated. For a function that is called many times, this can greatly reduce the amount of derivative information that must be stored.

In this chapter, we investigate how to write and debug adjoint code. To begin, we investigate how to write adjoint code for a simple function that takes 1–4 independent variables and returns 1 dependent variable. The adjoint code for such functions is simpler to write than that for a general function—such as the singular value decomposition of a matrix, which we will consider later.

13.2 Writing adjoint code: a simple case

Consider a simple function f which takes 1 independent variable x and returns a dependent variable y, i.e.,

$$y = f(x)$$

where $f(x) = \exp(-x^2/2)$. The code for this example can be written like

```
dvariable errf(const prevariable& x)
{
  return exp(-0.5*square(x));
}
```

There are three arithmetic operations here: square, multiplication, and exponentiation, so 96 bytes of derivative information will be generated. (Actually, the `return` operation also generates 32 bytes of derivative information, but we will ignore that for now.) A less efficient way to write the code (but more useful for showing adjoint code for this simple example) would be:

```
dvariable errf(const prevariable& x)
{
  dvariable y;
  y=exp(-0.5*square(x));
  return y;
}
```

Here is the same code with the derivative calculated by the one line of adjoint code `double dfx=-value(x)*value(y);`:

```
dvariable errf(const prevariable& x)
{
  dvariable y;
  value(y)=exp(-0.5*square(value(x)));
  double dfx=-value(x)*value(y);
  AD_SET_DERIVATIVES(y,x,dfx); // 1 dependent variable
  return y;
}
```

So what is going on here? Consider the line

```
value(y)=exp(-0.5*square(value(x)));
```

The `value` function returns a constant type, that is, a double, that has the same value as the corresponding `dvariable` or prevariable. In fact, it is the *same* object. That is, it shares the same address, but the type has been changed to double. So, the above line of code assigns the value `exp(-0.5*square(value(x)))` to `y`, but without generating any derivative code. Similarly, since the calculations are made on `value(x)`, these calculations will not generate any derivative code. So, it is the responsibility of the programmer to calculate the derivative code and store it where it can be used later. The line

```
double dfx=-value(x)*value(y);
```

calculates the derivative $f'(x)$ of y with respect to x and stores it with the line of code

```
AD_SET_DERIVATIVES(y,x,dfx);
```

This code will only generate 32 bytes of derivative information.

13.3 Debugging adjoint code: a simple case

The simplest way to debug the adjoint code is to put your new function into an AD Model Builder template file and use the `-dd 1` command line option to call the derivative checker.

```
DATA_SECTION
PARAMETER_SECTION
  init_number x
 !! x=2;
  objective_function_value f;
PROCEDURE_SECTION
  f=square(errf(x);

GLOBALS_SECTION
  #include <admodel.h>
  dvariable errf(const prevariable& x)
  {
    dvariable y;
    value(y)=exp(-0.5*square(value(x)));
    double dfx=-value(x)*value(y);
    AD_SET_DERIVATIVES(y,x,dfx); // 1 dependent variable
    return y;
  }
```

13.4 Adjoint code for more than one independent variable

The following code shows how to write the adjoint code for a function with two independent variables:

```
DATA_SECTION
  vector lengths(1,10)
  vector ages(1,10)
  !! lengths.fill_seqadd(1,1);
  !! ages.fill_seqadd(1,1);
  !! lengths=sqrt(lengths);

PARAMETER_SECTION
  init_bounded_number linf(0,10)
  init_bounded_number rho(0,1)
  objective_function_value f;
PROCEDURE_SECTION
  for (int i=1;i<=10;i++)
    f+=square(lengths(i)-vb_growth(linf,rho,ages(i)));

GLOBALS_SECTION
  #include <admodel.h>
```

```
  dvariable vb_growth(const prevariable& linf, const prevariable& rho,
    double t)
  {
    double clinf=value(linf);
    double crho=value(rho);
    dvariable len;
    value(len)=clinf*(1-pow(crho,t));
    double dflinf=1-pow(crho,t);
    double dfrho=-clinf*t*pow(crho,t-1);
    AD_SET_DERIVATIVES2(len,rho,dfrho,linf,dflinf); // 3 dependent variable
    return len;
  }
```

This approach to writing adjoint code has been implemented for functions of up to four independent variables.

```
DATA_SECTION
  vector lengths(1,10)
  vector ages(1,10)
  !! lengths.fill_seqadd(1,1);
  !! ages.fill_seqadd(1,1);
  !! lengths=sqrt(lengths);

PARAMETER_SECTION
  init_bounded_number linf(0,10)
  init_bounded_number rho(0,1)
  init_number t0
  init_bounded_number gamma(.1,1.9)
  objective_function_value f;
PROCEDURE_SECTION
  for (int i=1;i<=10;i++)
    f+=square(lengths(i)-vb_growth(linf,rho,t0,gamma,ages(i)));

GLOBALS_SECTION
  #include <admodel.h>

  dvariable vb_growth(const prevariable& linf, const prevariable& rho,
    const prevariable& t0, const prevariable gamma,double t)
  {
    double clinf=value(linf);
    double ct0=value(t0);
    double crho=value(rho);
    double cgamma=value(gamma);
```

```
  dvariable len;
  value(len)=pow(clinf*(1-pow(crho,t-ct0)),cgamma);
  double tmp=cgamma*pow(clinf*(1-pow(crho,t-ct0)),cgamma-1);
  double dflinf=tmp*(1-pow(crho,t-ct0));
  double dft0=tmp*(clinf*log(crho)*pow(crho,t-ct0));
  double dfrho=-tmp*clinf*(t-ct0)*pow(crho,t-ct0-1);
  double dfgamma=value(len)*log(clinf*(1-pow(crho,t-ct0)));
  AD_SET_DERIVATIVES4(len,t0,dft0,rho,dfrho,linf,dflinf,gamma,dfgamma);
    // 4 dependent variable
  return len;
}
```

13.5 Structured calculation of derivatives in adjoint code

Until now, we have deliberately calculated the derivatives with respect to the independent variables in an *ad-hoc* fashion. While this approach works for simple functions, it rapidly becomes untenable when the function is more complicated. In the following example, we have calculated the derivatives in a more structured fashion. Notice that to calculate the derivatives, every line of code in the function is repeated in the opposite order (commented out, of course) and the corresponding derivatives are calculated.

```
DATA_SECTION
  vector lengths(1,10)
  vector ages(1,10)
  !! lengths.fill_seqadd(1,1);
  !! ages.fill_seqadd(1,1);
  !! lengths=sqrt(lengths);

PARAMETER_SECTION
  init_bounded_number linf(0,10)
  init_bounded_number rho(0,1)
  init_number t0
  init_bounded_number gamma(.1,1.9)
  objective_function_value f;
PROCEDURE_SECTION
  for (int i=1;i<=10;i++)
    f+=square(lengths(i)-vb_growth(linf,rho,t0,gamma,ages(i)));

GLOBALS_SECTION
  #include <admodel.h>

  dvariable vb_growth(const prevariable& linf, const prevariable& rho,
```

```
  const prevariable& t0, const prevariable gamma,double t)
{
  double clinf=value(linf);
  double ct0=value(t0);
  double crho=value(rho);
  double cgamma=value(gamma);
  dvariable len;
  double u1=pow(crho,t-ct0);
  double u2=clinf*(1-u1);
  value(len)=pow(u2,cgamma);
  double dflen=1.0;
  //value(len)=pow(u2,cgamma);
  double dfu2=dflen*cgamma*pow(u2,cgamma-1.0);
  double dfgamma=dflen*value(len)*log(u2);
  //double u2=clinf*(1-u1);
  double dflinf=dfu2*(1-u1);
  double dfu1=-dfu2*clinf;
  //double u1=pow(crho,t-ct0);
  double dfrho=dfu1*(t-ct0)*pow(crho,t-ct0-1.0);
  double dft0=-dfu1*u1*log(crho);

  AD_SET_DERIVATIVES4(len,t0,dft0,rho,dfrho,linf,dflinf,gamma,dfgamma);
    // 4 dependent variable
  return len;
}
```

13.6 General adjoint code

So far, the adjoint code has been for a simple function which has from 1 to 4 independent variables and returns 1 dependent variable. Now we consider the general case where the function can take any number of dependent variables and return any number of dependent variables, and these variables can be in the form of numbers, vectors, or matrices.

```
dvar_vector operator * (_CONST dvar_matrix& m,_CONST dvar_vector& x )
{
  if (x.indexmin() != m.colmin() || x.indexmax() != m.colmax())
  {
    cerr << " Incompatible array bounds in dvar_vector operator * "
          << "(_CONST dvar_matrix& m,_CONST dvar_vector& x)\n";
    ad_exit(21);
  }
```

```
  dvar_vector tmp(m.rowmin(),m.rowmax());
  double sum;

  for (int i=m.rowmin(); i<=m.rowmax(); i++)
  {
    sum=0.0;
    for (int j=x.indexmin(); j<=x.indexmax(); j++)
    {
      sum+=(m.elem(i)).elem_value(j)*x.elem_value(j);
    }
    tmp.elem_value(i)=sum;
  }
 save_identifier_string("PLACE4");
 x.save_dvar_vector_value();
 x.save_dvar_vector_position();
 save_identifier_string("PLACE3");
 m.save_dvar_matrix_value();
 m.save_dvar_matrix_position();
 save_identifier_string("PLACE2");
 tmp.save_dvar_vector_position();
 save_identifier_string("PLACE1");

 ADJOINT_CODE(dmdv_prod);
  return(tmp);
}
```

To calculate the adjoint code, it will be necessary to have the values of the matrix `m` and the vector `x`. This is accomplished with the instructions

```
 x.save_dvar_vector_value();
 m.save_dvar_matrix_value();
```

Also, to calculate the derivatives, it will be necessary to know where the derivatives with respect to the independent and dependent variables are located. This information is saved with the instructions

```
 x.save_dvar_vector_position();
 m.save_dvar_matrix_position();
 tmp.save_dvar_vector_position();
```

Finally, we need to save the name of the routine that calculates the adjoint code, so that it can be called at the appropriate time. To write the code for the adjoint calculations, keep in mind that everything must be recovered from the stack in the reverse order from which it was put on the stack. This process can be a bit confusing and if you don't do it properly, the stack will become corrupted and nothing will work. To help diagnose problems, function `save_identifier_string` can be used to put a string on the stack. This string value can be

checked in the adjoint code with the `verify_identifier_string` function. At least two of these functions should be left in any adjoint code, so that stack integrity can be monitored if problems show up later. For optimized code, they are not used, and so contribute almost nothing to the overhead.

The adjoint code begins by reading the information that was saved on the stack. An object of type `dvar_vector_position` contains both the size and address information associated with a `dvar_vector`—which are needed to recover or store derivative values, or to build a `dvector` with the same shape as the $\widehat{\text{dvar\_vector}}$. The function `restore_dvar_vector_derivatives` gets the values of the derivatives with respect to the dependent variables, so they can be used in the adjoint code. The functions

```
dfx.save_dvector_derivatives(x_pos);
dfm.save_dmatrix_derivatives(m_pos);
```

use the position information to save the derivatives with respect to the independent variables in the appropriate places.

```
void dmdv_prod(void)
{
  verify_identifier_string("PLACE1");
  dvar_vector_position tmp_pos=restore_dvar_vector_position();
  verify_identifier_string("PLACE2");
  dvar_matrix_position m_pos=restore_dvar_matrix_position();
  dmatrix m=restore_dvar_matrix_value(m_pos);
  verify_identifier_string("PLACE3");
  dvar_vector_position x_pos=restore_dvar_vector_position();
  dvector x=restore_dvar_vector_value(x_pos);
  verify_identifier_string("PLACE4");
  dvector dftmp=restore_dvar_vector_derivatives(tmp_pos);

  dmatrix dfm(m_pos);
  dvector dfx(x_pos.indexmin(),x_pos.indexmax());
  dfm.initialize();
  dfx.initialize();

   double dfsum;
   for (int i=m.rowmax(); i>=m.rowmin(); i--)
   {
     // tmp.elem_value(i)=sum;
     dfsum=dftmp.elem(i);
     for (int j=x.indexmax(); j>=x.indexmin(); j--)
     {
       //sum+=(m.elem(i)).elem_value(j)*x.elem_value(j);
       dfm.elem(i,j)+=dfsum*x.elem(j);
```

```
      dfx.elem(j)+=dfsum*m.elem(i,j);
    }
    //sum=0.0;
    dfsum=0.0;
  }
  dfx.save_dvector_derivatives(x_pos);
  dfm.save_dmatrix_derivatives(m_pos);
}
```

Chapter 14

Truncated Regression

14.1 Truncated linear regression

The linear regression model we consider here has the form

$$Y_i = \sum_{j=1}^{m} a_j x_{ij} + \epsilon_i$$

where the Y_i for $i = 1, \ldots, n$ are the n observations and the a_j are m parameters to be estimated. The ϵ_i are assumed to be normally distributed random variables with mean 0 and variance v.

Let $r_i = Y_i - \sum_{j=1}^{m} a_j x_{ij}$. The log-likelihood function for the standard regression model is given by

$$-.5n \log(v) - \sum_{i=1}^{n} \frac{r_i^2}{2v}$$

Now assume that we only consider the Y_i for $Y_i \geq 0$, i.e., the left truncated situation. The probability that $Y_i \geq 0$ is equal to the probability that $\epsilon_I > -\sum_{j=1}^{m} a_j x_{ij}$. This is equal to $1 - \Phi(-\sum_{j=1}^{m} a_j x_{ij}/v)$, where

$$\Phi(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{u} \exp\left(-t^2/2\right) \, \mathrm{d}t$$

For this truncated regression, the log-likelihood function has the logarithm of this quantity subtracted from it, so it becomes

$$-.5n \log(v) - \sum_{i=1}^{n} \frac{r_i^2}{2v} - \log\left(1 - \Phi\Big(-\sum_{j=1}^{m} a_j x_{ij}/v\Big)\right)$$

If instead we consider the right truncated case, where only the $Y_i < 0$ are considered, the log-likelihood function becomes

$$-.5n \log(v) - \sum_{i=1}^{n} \frac{r_i^2}{2v} - \log\left(\Phi\Big(-\sum_{j=1}^{m} a_j x_{ij}/v\Big)\right)$$

To parameterize v, we introduce a new parameter a satisfying the condition $v = a\hat{v}$, where $\hat{v} = \frac{1}{n}\sum_{i=1}^{n} r_i^2$ is the usual maximum likelihood estimate for v. This leads to more numerically stable behavior. In terms of a, the expression for the log-likelihood simplifies to

$$-.5n\log(a) - .5n\log(\hat{v}) - \frac{n}{2a} - \log\left(1 - \Phi\left(-\sum_{j=1}^{m} a_j x_{ij}/(a\hat{v})\right)\right)$$

14.2 The AD Model Builder truncated regression program

Here are the contents of the file `truncreg.tpl`:

```
DATA_SECTION
  init_int nobs
  init_int m
  init_int trunc_flag
  init_matrix data(1,nobs,1,m+1)
  vector Y(1,nobs)
  matrix X(1,nobs,1,m)
 LOC_CALCS
  Y=column(data,1);
  for (int i=1;i<=nobs;i++)
  {
    X(i)=data(i)(2,m+1).shift(1);
  }
PARAMETER_SECTION
  sdreport_number sigma
  number vhat
  init_bounded_number log_a(-5.0,5.0);
  sdreport_number a
  init_vector u(1,m)
  objective_function_value f
PROCEDURE_SECTION
  a=exp(log_a);
  dvar_vector pred=X*u;
  dvar_vector res=Y-pred;
  dvariable r2=norm2(res);
  vhat=r2/nobs;
  dvariable v=a*vhat;
  sigma=sqrt(v);

  dvar_vector spred=pred/sigma;
```

```
  f=0.0;
  switch (trunc_flag)
  {
  case -1: // left_truncated
    {
      for (int i=1;i<=nobs;i++)
      {
        f+=log(1.00001-cumd_norm(-spred(i)));
      }
    }
    break;
  case 1:  // right truncated
    {
      for (int i=1;i<=nobs;i++)
      {
        f+=log(0.99999*cumd_norm(-spred(i)));
      }
    }
    break;
  case 0:  // no truncation
    break;
  default:
    cerr << "Illegal value for truncation flag" << endl;
    ad_exit(1);
  }
  f+=0.5*nobs*log(v)+0.5*r2/v;


REPORT_SECTION
  report << "#u " << endl << u << endl;
  report << "#sigma " << endl << sigma << endl;
  report << "#a " << endl << a << endl;
  report << "#vhat " << endl << vhat << endl;
  report << "#shat " << endl << sqrt(vhat) << endl;
```

Chapter 15

All the Functions in AD Model Builder

This chapter attempts to list and document all the functions available in AD Model Builder. It will always be incomplete, since functions are continually being added. If you are aware of a function that is not documented please, contact me at otter@otter-rsch.com and let me know.

15.1 Naming conventions for documenting functions

Wherever applicable, the `name` function has been supplied for constant and variable objects (such as `double` and `dvariable`). Instead of repeating the description for both kinds of objects, the convention of referring to both types as "number," "vector," "matrix," etc., will be observed.

15.2 Mathematical functions

The following functions have been included in AUTODIF, by overloading the C++ library functions or adding additional functions where necessary:

```
acos atan cos cosh cube exp (mfexp) fabs gammln (sfabs) log log_comb
log10 log_density_poisson pow square sqrt sin sinh tan tanh
```

These functions can be used on `number`s or `vector_object`s in the form

```
number = function(number);
vector_object = function(vector_object);
```

When operating on `vector_object`s, the functions operate elemen-by-element, so if `y` is a `dvector` whose elements are $(y_1, \ldots, y_n)$, then `exp(y)` is a `dvector` whose elements are $(\exp(y_1), \ldots, \exp(y_n))$.

The functions `min` and `max`, when applied to a `vector_object`, return a `number` that is equal to the minimum or maximum element of the `vector_object`.

The function `gammln` is the logarithm of the gamma function.

The function `log_comb(n,k)` is the logarithm of the function, the combination of `n` things taken `k` at a time. It is defined via the logarithm of the gamma function for non-integer values, and is differentiable.

15.3 Operations on arrays

15.3.1 Element-wise operations

There are several operations familiar to users of spreadsheets that do not appear as often in classical mathematical calculations. For example, spreadsheet users often wish to multiply one column in a spreadsheet by the corresponding elements of another column. Spreadsheet users might find it much more natural to define the product of matrices as an element-wise operation, such as

$$z_{ij} = x_{ij} * y_{ij}$$

The "classical" mathematical definition for the matrix product has been assigned to the overloaded operator '`*`,' so large mathematical formulas involving vector and matrix operations can be written in a concise notation. Typically, spreadsheet-type calculations are not so complicated and do not suffer so much from being forced to adopt a "function style" of notation.

Since addition and subtraction are already defined in an element-wise manner, it is only necessary to define element-wise operations for multiplication and division. We have named these functions `elem_prod` and `elem_div`.

`vector_object = elem_prod(vector_object,vector_object)` *`// element-wise multiply`*
$z_i = x_i * y_i$

`vector_object = elem_div(vector_object,vector_object)` *`// element-wise divide`*
$z_i = x_i / y_i$

`matrix_object = elem_prod(matrix_object,matrix_object)` *`// element-wise multiply`*
$z_{ij} = x_{ij} * y_{ij}$

`matrix_object = elem_div(matrix_object,matrix_object)` *`// element-wise divide`*
$z_{ij} = x_{ij} / y_{ij}$

15.4 The identity matrix function `identity_matrix`

`matrix_object = identity_matrix(int min,int max)`
creates a square identity matrix with minimum valid index `min` and maximum valid index `max`.

15.5 Probability densities and related functions: `poisson negative binomial cauchy`

`number log_density_cauchy(number x);`
returns the logarithm of the Cauchy density function at `x`.

`number log_density_poisson(number x,number mu);`
returns the logarithm of the Poisson density function at `x` with mean `mu`.

`number log_negbinomial_density(number x,number mu,number tau);`
returns the logarithm of the negative binomial density function with mean `mu` and over-dispersion (variance/mean) `tau`. `tau` must be greater than 1.

15.6 The operations `det inv norm norm2 min max sum`

The determinant of a matrix object

(The matrix must be square, that is, the number of rows must equal the number of columns.)

```
matrix_object = det(matrix_object)
```

The inverse of a matrix object

(The matrix must be square, that is, the number of rows must equal the number of columns.)

```
matrix_object = inv(matrix_object)
```

The norm of a vector object

```
number = norm(vector_object)
```
$z = \sqrt{\sum_i x_i^2}$

The norm squared of a vector object

```
number = norm2(vector_object)
```
$z = \sum_i x_i^2$

The norm of a matrix object

```
number = norm(matrix_object)
```
$z = \sqrt{\sum_{ij} x_{ij}^2}$

The norm squared of a matrix object

`number = norm2(matrix_object)`
$z_{ij} = x_{ji}$

The transpose of a matrix object

`matrix_object = trans(matrix_object)`
$z = \sum_{ij} x_{ij}^2$

The sum over the elements of a vector object

`number = sum(vector_object)`
$z = \sum_i x_i$

The row sums of a matrix object

`vector = rowsum(matrix_object)`
$z_i = \sum_j x_{ij}$

The column sums of a matrix object

`vector = colsum(matrix_object)`
$z_j = \sum_i x_{ij}$

The minimum element of a vector object

`number = min(vector_object)`

The maximum element of a vector object

`number = max(vector_object)`

15.7 Eigenvalues and eigenvectors of a symmetric matrix

While we have included eigenvalue and eigenvector routines for both constant and variable matrix objects, you should be aware that, in general, the eigenvectors and eigenvalues are not differentiable functions of the variables determining the matrix.

`matrix_object = eigenvectors(matrix_object)`
returns in a matrix the eigenvectors of a symmetric matrix.

It is the user's responsibility to ensure that the matrix is actually symmetric. The routine symmetrizes the matrix, so the eigenvectors returned are actually those for the symmetrized matrix. The eigenvectors are located in the columns of the matrix. The i^{th} eigenvalue returned by the function `eigenvalues` corresponds to the i^{th} eigenvector returned by the function `eigenvectors`.

15.8 The Choleski decomposition of a positive definite symmetric matrix

For a positive definite symmetric matrix `S`, the Choleski decomposition of `S` is a lower triangular matrix `T` satisfying the relationship `S=T*trans(T)`. If `S` is a (positive definite symmetric) matrix object and `T` is a matrix object, the line of code

```
T=choleski_decomp(S);
```

will calculate the Choleski decomposition of `S` and put it into `T`.

15.9 Solving a system of linear equations

If `y` is a vector and `M` is an invertible matrix, then finding a vector `x` such that

```
x=inv(M)*y
```

will be referred to as "solving the system of linear equations determined by `y` and `M`." Of course, it is possible to use the `inv` function to accomplish this task, but it is much more efficient to use the `solve` function:

```
vector x=solve(M,y); // x will satisfy x=inv(M)*y;
```

It turns out that it is a simple matter to calculate the determinant of the matrix `M` while solving the system of linear equations. Since this is useful in multivariate analysis, we have also included a function that returns the determinant when the system of equations is solved. To avoid floating point overflow, or underflow when working with large matrices, the logarithm of the absolute value of the determinant, together with the sign of the determinant, are returned. The constant form of the `solve` function is

```
double ln_det;
double sign;
dvector x=solve(M,y,ln_det,sign);
```

while the variable form is

```
dvariable ln_det;
dvariable sign;
dvar_vector x=solve(M,y,ln_det,sign);
```

The `solve` function is useful for calculating the log-likelihood function for a multivariate normal distribution. Such a log-likelihood function involves a calculation similar to

```
l = -.5*log(det(S)) -.5*y*inv(S)*y
```

where `S` is a matrix object and `y` is a vector object. It is much more efficient to carry out this calculation using the `solve` function. The following code illustrates the calculations for variable objects:

```
dvariable ln_det;
dvariable sign;
dvariable l;
dvar_vector tmp=solve(M,y,ln_det,sign);
l=-.5*ln_det-y*tmp;
```

15.10 Methods for filling arrays and matrices

While it is always possible to fill vectors and matrices by using loops and filling them element by element, this is tedious and prone to error. To simplify this task, a selection of methods for filling vectors and matrices with either random numbers, or a specified sequence of numbers, is available. There are also methods for filling row and columns of matrices with vectors. In this section, the symbol `vector` can refer to either a `dvector` or a `dvar_vector`, while the symbol `matrix` can refer to either a `dmatrix` or a `dvar_matrix`.

`void vector::fill("{m,n,...,}")`
fills a vector with a sequence of the form `n, m, ...` The number of elements in the string must match the size of the vector.

`void vector::fill_seqadd(double& base, double& offset)`
fills a vector with a sequence of the form `base, base+offset, base+2*offset,...`

For example, if `v` is a `dvector` created by the statement

```
dvector v(0,4);
```

then the statement

```
v.fill_seqadd(-1,.5);
```

will fill `v` with the numbers $(-1.0, -0.5, 0.0, 0.5, 1.0)$.

`void matrix::rowfill_seqadd(int& i,double& base, double& offset)`
fills row `i` of a matrix with a sequence of the form `base, base+offset, base+2*offset,...`

`void matrix::colfill_seqadd(int& j,double& base, double& offset)`
fills column `j` of a matrix with a sequence of the form `base, base+offset, base+2*offset,...`

`void matrix::colfill(int& j,vector&)`
fills the j^{th} column of a matrix with a vector.

`void matrix::rowfill(int& i,vector&)`
fills the i^{th} row of a matrix with a vector.

15.11 Methods for filling arrays and matrices with random numbers

This method of filling containers with random numbers is becoming obsolete. The preferred method is to use the `random_number_generator` class. See Section 15.17 for instructions on using this class. In this section, a uniformly distributed random number is assumed to have a uniform distribution on $[0, 1]$. A normally distributed random number is assumed to have mean 0 and variance 1. A binomially distributed random number is assumed to have a parameter p, where 1 is returned with probability p, and 0 is returned with probability $1-p$. A multinomially distributed random variable is assumed to have a vector of parameters P, where i is returned with probability p_i. If the components of P do not sum to 1, the vector will be normalized so that the components *do* sum to 1.

`void vector::fill_randu(long int& n)`
fills a vector with a sequence of uniformly distributed random numbers. The `long int n` is a seed for the random number generator. Changing `n` will produce a different sequence of random numbers. *This function is now obsolete. You should use the* `random_number_generator` *class to generate random numbers.*

`void matrix::colfill_randu(int& j,long int& n)`
fills column `j` of a matrix with a sequence of uniformly distributed random numbers The `long int n` is a seed for the random number generator. Changing `n` will produce a different sequence of random numbers.

`void matrix::rowfill_randu(int& i,long int& n)`
fills row `i` of a matrix with a sequence of uniformly distributed random numbers.

`void vector::fill_randbi(long int& n, double& p)`
fills a vector with a sequence of random numbers from a binomial distribution.

`void vector::fill_randn(long int& n)`
fills a vector with a sequence of normally distributed random numbers. *This function is now obsolete. You should use the* `random_number_generator` *class to generate random numbers.*

`void matrix::colfill_randn(int& j,long int& n)`
fills column `j` of a matrix with a sequence of normally distributed random numbers.

`void matrix::rowfill_randn(int& i,long int& n)`
fills row `i` of a matrix with a sequence of normally distributed random numbers.

`void vector::fill_multinomial(long int& n, dvector& p)`
fills a vector with a sequence random numbers from a multinomial distribution. The parameter p is a `dvector` such that `p[i]` is the probability of returning i. The elements of `p` must sum to 1.

15.12 Methods for obtaining shape information from containers

When this code was first written, the maximum dimension of arrays was about four. At this level, it perhaps make sense to think of a 1-dimensional array as a vector, a 2-dimensional array as a matrix, etc. For a matrix, one thinks in terms of rows and columns. However, with the adoption of ragged container objects up to eight dimensions (at present), a more generic method of obtaining shape information of these objects was called for.

If `v` is a vector object, then

```
int v.indexmin()
int v.indexmax()
```

return the minimum and maximum valid indices for `v`. If `m` is a matrix object, then

```
int v.rowmin()
int v.rowmax()
int v.colmin()
int v.colmax()
```

return the minimum and maximum valid row and column indices for `m`. These functions make sense for a matrix where every row is a vector with the same minimum and maximum valid indices. For a ragged matrix, this is no longer the case, so the `rowmin()` and `rowmax()` functions don't make sense. To deal with a ragged matrix, one may need to calculate the minimum and maximum valid indices for each row of the ragged matrix. To facilitate this approach, the functions `indexmin` and `indexmax` have been defined for all container classes. So, for example, if `w` is a 6-dimensional array, then

```
int w.indexmin()
int w.indexmax()
```

return the minimum and maximum valid indices for the first index of `w`. For a matrix object `m`, `m.indexmin()` and `m.colmin()` are the same and as long as `m` is not ragged,

```
m(m.indexmin()).indexmin()
```

is the same as

```
m.colmin()
```

and

```
m(m.indexmin()).indexmax()
```

is the same as

```
m.colmax()
```

15.13 Methods for extracting from arrays and matrices

`vector column(matrix& M,int& j)`
extracts the j^{th} column from a matrix and puts it into a vector.

`vector extract_row(matrix& M,int& i)`
extracts a row from a matrix and puts it into a vector. Note that the operation `M(i)` has the same effect.

`vector extract_diagonal(matrix& M)`
extracts the diagonal elements from a matrix and puts them into a vector.

The function call operator `()` has been overloaded in two ways to provide for the extraction of a subvector.

```
vector(ivector&)
```

An `ivector` object is used to specify the elements of the vector to be chosen. If `u` and `v` are `dvectors` and `i` is an `ivector`, the construction

```
dvector u = v(i);
```

will extract the members of `v` indexed by `i` and put them in the `dvector u`. The size of `u` is equal to the size of `i`. The `dvector u` will have minimum valid index and maximum valid index equal to the minimum valid index and maximum valid index of `i`. The size of `i` can be larger than the size of `v`, in which case some elements of `v` must be repeated. The elements of the `ivector i` must lie in the valid index range for `v`.

If `v` is a `dvector` and `i1` and `i2` are two integers,

```
u(i1,i2)
```

is a `dvector`, which is a subvector of `v` (provided, of course, that `i1` and `i2` are valid indices for `v`). Subvectors can appear on both the left and right hand side of an assignment:

```
dvector u(1,20);
dvector v(1,19);
v = 2.0;  // assigns the value 2 to all elements of v
u(1,19) = v; // assigns the value 2 to elements 1 through 19 of u
```

In the above example, suppose that we wanted to assign the vector `v` to elements 2 through 20 of the vector `u`. To do this, we must first ensure that they have the same valid index ranges. The operators `++` and `--` increment and decrement the index ranges by 1.

```
dvector u(1,20);
dvector w(1,19);
dvector v(1,19);

v = 2.0;  // assigns the value 2 to all elements of v
```

```
--u(2,20) = v; // assigns the value 2 to elements 2 through 20 of u

u(2,20) = ++v; // assigns the value 2 to elements 2 through 20 of u
               // probably not what you want
w=v;  // error different index ranges
```

It is important to realize that from the point of view of the vector `u`, both of the above assignments have the same effect. It will have elements 2 through 20 set equal to 2. The difference is in the side effects on the vector `v`. The operation `++v` will increase the minimum and maximum valid index range of the vector `v` by 1. This increase is permanent. On the other hand, the operation `--u(2,20)` decrements the valid index bounds of the *subvector* `u(2,20)`. This is a distinct object from the vector `u`, although both objects share a common area for their components. Thus, the valid index bounds of `u` are not affected by this process. The use of subvectors, along with increment and decrement operations, can be used to remove loops from the code. Note that

```
dvector x(1,n)
dvector y(1,n)
dvector z(1,n)
for (int i=2;i<=n;i++)
{
  x(i)=y(i-1)*z(i-1);
}
```

can be written as

```
dvector x(1,n)
dvector y(1,n)
dvector z(1,n)
x(2,n)=++elem_prod(y(1,n-1),z(1,n-1)); // elem_prod is element-wise
                                       // multiplication of vectors
```

The `shift` function can be used to set the minimum (and maximum) valid index for a vector.

```
dvector u(10,100); // minimum valid index is 10
                   // maximum valid index is 100
u.shift(25);       // minimum valid index is 25
                   // maximum valid index is 115
```

In particular, the operators `--` and `++` are just convenient shorthand for using the `shift` function to change the minimum valid index by 1.

```
dvector u(10,100);   // minimum valid index is 10
                     // maximum valid index is 100
u.shift(u.indexmin()-1); // minimum valid index is 9
--u;                 // same result as u.shift(u.indexmin()-1)
```

```
u.shift(u.indexmin()+1); // minimum valid index is 11
++u;                     // same result as u.shift(u.indexmin()+1)
```

15.14 Accessing subobjects of higher-dimensional arrays

The `()` operator cannot be used to access subobjects of arrays of dimension 2 or greater, because this operator has already been defined to do something else. For example, for a `dmatrix M`, `M(1,2)` is an *element* of `M`. To access subobjects of higher-dimensional arrays, use the `sub` member function. If `M` is a matrix object, then `M.sub(2,6)` is a matrix object with minimum valid index 2 and maximum valid index 6 (provided, of course, that the minimum valid index for `M` is less than or equal to 2 and the maximum valid index is greater than or equal to 6). If `T` is a 3-dimensional object, then `T.sub(2,5)` is a 3-dimensional object, provided that the index bounds are legal.

15.15 Sorting vectors and matrices

While sorting is not strictly a part of methods for calculating the derivatives of differentiable functions (it is a highly non-differentiable operation), it is so useful for pre and post-processing data that we have included some functions for sorting `dvector` and `dmatrix` objects. If `v` is a `dvector` the statement

```
dvector w=sort(v);
```

will sort the elements of `v` in ascending order and put them in the `dvector` object `w`. The minimum and maximum valid indices of `w` will be the same as those of `v`. If desired, an index table for the sort can be constructed by passing an `ivector` along with the `dvector`. This index table can be used to sort other vectors in the same order as the original vector by using the `()` operator.

```
dvector u={4,2,1};
dvector v={1,6,5}
ivector ind(1,3);
dvector w=sort(u,ind); // ind will contain an index table for the sort
// Now w=(1,2,4) and ind=(3,2,1)
dvector ww=v(ind);   // This is the use of the ( ) operator for subset
                     // selection.
// Now ww=(5,6,1)
```

The `sort` function for a `dmatrix` object sorts the columns of the `dmatrix` into ascending order, using the column specified to do the sorting. For example,

```
dmatrix MM = sort(M,3);
```

will put the sorted matrix into `MM`, and the third column of `MM` will be sorted in ascending order.

15.16 Statistical functions

```
cumd_norm
inv_cumd_norm
cumd_cauchy
inv_cumd_cauchy
```

These are the cumulative distribution function and the inverse cumulative distribution function for the normal and Cauchy distributions.

15.17 The random number generator class

The random number generator class is used to manage the generation of random numbers. A random number generator object is created with the declaration

```
random_number_generator r(n);
```

where `n` is the seed that initializes the random number generator. Any number of random number generators may be declared. This class can be used to manage random number generation with the following functions:

```
randpoisson(lambda,r); // generate a Poisson with mean lambda
randnegbinomiual(mu,tau,r); // generate a negative binomial with mean mu
                        // and over-dispersion tau (tau>1)
randn(r);    // generate a normally distributed random number
randu(r);   // generate a uniformly distributed random number
v.fill_randu(r) // fill a vector v
v.fill_randn(r) // fill a vector v
v.fill_randpoisson(mu,r) // fill a vector v with Poisson distributed
                         // random variables with mean mu
v.fill_rand(mu,tau,r) // fill a vector v with negative binomial distributed
           // random variables with mean mu and over-dispersion var/mu = tau
v.fill_multinomial(r,p) // fill a vector v
                    // p is a vector of probabilities
m.fill_randu(r) // fill a matrix m
m.fill_randn(r) // fill matrix m
m.fill_randpoisson(lambda,r) // fill a matrix m
```

The incomplete beta function $I_x(a,b)$ is defined by

$$I_x(a,b) = \frac{1}{B(a,b)} \int_0^x t^{a-1}(1-t)^{b-1}\,\mathrm{d}t \qquad (a,b,>0) \tag{15.1}$$

This is also the cumulative distribution function for the beta family of probability distributions. The function is named `betai` and is invoked by

```
\\ .....
dvariable p=betai(a,b,x);
```

15.18 The adstring class operations

The adstring class was defined before there was a standardized C++ string class. It does not contain all the features that a full string class should have. It is, however, easier to use in many cases than the standard C string operations.

```
adstring s;
adstring t;
s="first_part";
t="second_part";
adstring u = s + " ___ " + t;
cout << u << endl;
```

should print out

```
first_part ___ second_part
```

The operation + concatenates two adstring objects. It can be used to concatenate C-style strings by first turning them into adstring objects, as in

```
adstring u = adstring("xxx") + adstring("yyy");
```

One can also append to a string with the += operator, as in

```
adstring u = "abc";
u += v;
adstring w = "abc";
w += 'f';
```

which adds the adstring object v to u and the character 'f' to w. It is also possible to cast an adstring object to a C-like char * string, as in

```
adstring u = "abc"
char * c = (char*)(u);
```

Then it may be used as you would use a C-like string.

15.19 Miscellaneous functions

posfun(x,eps,pen)
The posfun function constrains the argument x to be positive. For x > eps, it is the identity function.

The current source code for the posfun function appears below:

```
dvariable posfun(const dvariable&x,const double eps,dvariable& pen)
{
  if (x>=eps) {
    return x;
```

```
  } else {
    pen+=.01*square(x-eps);
    return eps/(2-x/eps);
  }
}
```

`mfexp(_CONST prevariable& x)`
The `mfexp` function is the exponential function that is modified for large values of its argument, to prevent floating point overflows.

The current source code for the `mfexp` function appears below:

```
dvariable mfexp(_CONST prevariable& x)
{
  double b=60;
  if (x<b)
  {
    return exp(x);
  }
  else
  {
    return exp(b)*(1.+2.*(x-b))/(1.+x-b);
  }
}
```

Chapter 16

Miscellaneous and Advanced Features of AD Model Builder

16.1 Using strings and labels in the TPL file

For purposes of this manual, a "label" is a string that does not have any blanks in it. Such strings can be read in from the `data` file using the `init_adstring` declaration, as in

```
DATA_SECTION
  init_adstring s
```

The DAT file should contain something like

```
# label to be read in
  my_model_data
```

When the program runs, the `adstring` object `s` should contain the string

```
  my_model_data
```

White space at the beginning is ignored and following white space terminates the input of the object.

Discussions of the various operations on `adstring` class members are found elsewhere in the manual.

16.2 Using other class libraries in AD Model Builder programs

A useful feature of C++ is its open nature. This means that the user can combine several class libraries into one program. In general, this simply involves including the necessary header files in the program and then declaring the appropriate class instances in the program. Instances of external classes can be declared in an AD Model Builder program in several ways. They can always be declared in the procedure or report section of the program as

local objects. It is sometimes desired to include instances of external classes in a more formal way into an AD Model Builder program. This section describes how to include them into the DATA_SECTION or PARAMETER_SECTION. After that, they can be referred to as though they were part of the AD Model Builder code (except for the technicalities to be discussed below).

AD Model Builder employs a strategy of late initialization of class members. The reason for this is to allow time for the user to carry out any calculations that may be necessary for determining parameter values, etc., that are used in the initialization of the object. Because of the nature of constructors in C++, this means that every object declared in the DATA_SECTION or the PARAMETER_SECTION must have a default constructor that takes no arguments. The actual allocation of the object is carried out by a class member function named allocate, which takes any desired arguments. Since external classes will not generally satisfy these requirements, a different strategy is employed for these classes. A pointer to the object is included in the appropriate AD Model Builder class. This pointer has the prefix pad_ inserted before the name of the object. The pointer to myobj would have the form pad_myobj.

```
!!CLASSfooclass myobj( ...)
```

The user can refer to the object in the code simply by using its name.

16.3 Using control files for bounded parameters

Bounded parameters defined in the procedure section take the following format:

```
init_bounded_number a(lb,ub,i_phz);
```

where lb is the lower bound, ub is the upper bound and i_phz is and integer representing the phase of estimation. There is also an option to pass a vector containing 3 elements set the lower and upper bounds and the phase of estimation. This is often desirable as this vector can be read in from the data file and does not require recompiling of the code to change the parameter bounds or the phase of estimation.

```
init_bounded_number a(luphz_vector);
```

This has also been implemented for the init_bounded_number_vector, where a matrix read in from the data section is used to set the lower and upper bounds of each element and phase of estimation. The following is a simple example implementing these new features.

```
DATA_SECTION
  init_int nobs;
  init_vector y(1,nobs);
  init_vector x(1,nobs);

  // Controls for parameters.
  init_vector a_lup(1,3);
```

```
  init_vector b_lup(1,3);
  init_vector sig_lup(1,3);

  init_matrix theta_lup(1,3,1,3);
PARAMETER_SECTION

  init_bounded_number a(a_lup);
  init_bounded_number b(b_lup);
  init_bounded_number sig(sig_lup);

  init_bounded_number_vector theta(theta_lup);
  objective_function_value f;

  vector y_hat(1,nobs);
  vector y2_hat(1,nobs);

INITIALIZATION_SECTION
  sig 1.0;

PROCEDURE_SECTION

  y_hat = a + b * x;
  y2_hat = theta(1) + theta(2)*x;
  f     = dnorm(y - y_hat, sig);
  f    += dnorm(y-y2_hat,theta(3));
```

And the input data file is here:

```
# number of observations
     10
# observed Y values
    1.4  4.7  5.1  8.3  9.0  14.5  14.0  13.4  19.2  18
# observed x values
    -1  0 1  2  3  4  5  6  7  8

#a_lup
-5  5  1
#b_lup
-10  10  1
#sig_lup
0.01  3.0  2
#theta_lup
# lower bound, upper bound, phase
-5  5  1
```

```
-10 10 1
0.01 5.0 2
```

Appendix A

The Regression Function

The `robust_regression` function calculates the log-likelihood function for the standard statistical model of independent normally distributed errors, with mean 0 and equal variance. The code is written in terms of AUTODIF objects, such as `dvariable` and `dvar_vector`. They are described in the AUTODIF user's manual.

```
dvariable regression(const dvector& obs,const dvar_vector& pred)
{
  double nobs=double(size_count(obs)); // get the number of
                                       // observations
  dvariable vhat=norm2(obs-pred); // sum of squared deviations
  vhat/=nobs;                     //mean of squared deviations
  return (.5*nobs*log(vhat));  //return log-likelihood value
}
```

Appendix B

AD Model Builder Types

The effect of a declaration depends on whether or not it occurs in the DATA_SECTION or in the PARAMETER_SECTION. Objects declared in the DATA_SECTION are constant, that is, like data. Objects declared in the PARAMETER_SECTION are variable, that is, like the parameters of the model that are to be estimated. Any objects that depend on variable objects must themselves be variables objects, that is, they are declared in the PARAMETER_SECTION and not in the DATA_SECTION.

In the DATA_SECTION, the prefix init_ indicates that the object is to be read in from the data file. In the PARAMETER_SECTION, the prefix indicates that the object is an initial parameter whose value will be used to calculate the value of other (non-initial) parameters. In the PARAMETER_SECTION, initial parameters will either have their values read in from a parameter file or will be initialized with their default initial values. The actual default values used can be modified in the INITIALIZATION_SECTION. From a mathematical point of view, objects declared with the init_ prefix are independent variables that are used to calculate the objective function being minimized.

The prefixes bounded_ and dev_ can only be used in the PARAMETER_SECTION. The prefix bounded_ restricts the numerical values that an object can take on to lie in a specified bounded interval. The prefix dev_ can only be applied to the declaration of vector objects. It has the effect of restricting the individual components of the vector object so that they sum to zero.

The prefix sdreport_ can only be used in the PARAMETER_SECTION. An object declared with this prefix will appear in the covariance matrix report. This provides a convenient method for obtaining estimates for the variance of any parameter that may be of interest. Note that the prefixes sdreport_ and init_ cannot both be applied to the same object. There is no need to do so, since initial parameters are automatically included in the standard deviations report. AD Model Builder also has 3 and 4-dimensional arrays. They are declared like

```
3darray dthree(1,10,2,20,3,10)
4darray df(1,10,2,20,3,10)
init_3darray dd(1,10,2,20,3,10) // data section only
```

Declaration	Type of object	Type of object
	in DATA_SECTION	in PARAMETER_SECTION
[init_]int	int	int
[init_][bounded_]number	double	dvariable
[init_][bounded_][dev_]vector	vector of doubles (dvector)	vector of dvariables(dvar_vector)
[init_][bounded_]matrix	matrix of doubles (dmatrix)	matrix of dvariables(dvar_matrix)
[init_]3darray	3-dimensional array of doubles	3-dimensional array of dvariables
4darray	4-dimensional array of doubles	4-dimensional array of dvariables
5darray	5-dimensional array of doubles	5-dimensional array of dvariables
6darray	6-dimensional array of doubles	6-dimensional array of dvariables
7darray	7-dimensional array of doubles	7-dimensional array of dvariables
sdreport_number	N/A	dvariable
likeprof_number	N/A	dvariable
sdreport_vector	N/A	vector of dvariables(dvar_vector)
sdreport_matrix	N/A	matrix of dvariables(dvar_matrix)

Table B.1

```
init_4darray dxx(1,10,2,20,3,10) // data section only
```

Table B.1 contains a summary of declarations and the types of objects associated with them in AD Model Builder. The types `dvariable, dvector, dmatrix, d3_array, dvar_vector, dvar_matrix`, and `dvar3_array` are described in the AUTODIF user's manual.

Appendix C

The Profile Likelihood

We have been told that the profile likelihood as calculated in AD Model Builder for dependent variables may differ from that calculated by other authors. This section will clarify what we mean by the term and motivate our calculation.

Let $(x_1, \ldots, x_n)$ be n independent variables, $f(x_1, \ldots, x_n)$ be a probability distribution, and g denote a dependent variable that is a real valued function of $(x_1, \ldots, x_n)$. Fix a value g_0 for g and consider the integral

$$\int_{\{x: g_0 - \epsilon/2 \le g(x) \le g_0 + \epsilon/2\}} f(x_1, \ldots, x_n)$$

which is the probability that $g(x)$ has a value between $g_0 - \epsilon/2$ and $g_0 + \epsilon/2$. This probability depends on two quantities: the value of $f(x)$ and the thickness of the region being integrated over. We approximate $f(x)$ by its maximum value $\hat{x}(g) = \max_{x:g(x)=g_0}\{f(x)\}$. For the thickness, we have $g(\hat{x} + h) \approx g(\hat{x}) + \langle \nabla g(\hat{x}), h \rangle = \epsilon/2$, where h is a vector perpendicular to the level set of g at $\hat{x}$. However, ∇g is also perpendicular to the level set, so $\langle \nabla g(\hat{x}), h \rangle = \|\nabla g(\hat{x})\| \|h\|$, so in turn, $\|h\| = \epsilon/(2\|g(\hat{x})\|)$. Thus, the integral is approximated by $\epsilon f(\hat{x})/\|\nabla g(\hat{x})\|$. Taking the derivative with respect to ϵ yields $f(\hat{x})/\|\nabla g(\hat{x})\|$, which is the profile likelihood expression for a dependent variable.

Appendix D

Concentrated Likelihoods

The log-likelihood function for a collection of n observations Y_i, where the Y_i are assumed to be normally distributed random variables with mean μ and variance σ^2, has the form

$$-n\log(\sigma) - \sum_{i=1}^{n} \frac{(Y_i - \mu_i)^2}{2\sigma^2} \tag{D.1}$$

To find the maximum of this expression with respect to σ, take the derivative of expression (D.1) with respect to σ and set the resulting equation equal to zero.

$$-n/\sigma + \sum_{i=1}^{n} \frac{(Y_i - \mu_i)^2}{\sigma^3} = 0 \tag{D.2}$$

Solving equation (D.2) for $\hat{\sigma}^2$ yields

$$\hat{\sigma}^2 = 1 \Big/ n\sum_{i=1}^{n}(Y_i - \mu_i)^2 \tag{D.3}$$

Substituting this value into expression (D.1) yields

$$-.5n\log\left(\sum_{i=1}^{n}(Y_i - \mu_i)^2\right) + \text{const} \tag{D.4}$$

where "const" is a constant that can be ignored. It follows that maximizing expression (D.1) is equivalent to maximizing

$$-.5n\log\left(\sum_{i=1}^{n}(Y_i - \mu_i)^2\right) \tag{D.5}$$

Expression D.5 is referred to as the "concentrated log-likelihood."

See [6] for more complicated examples of concentrated likelihoods.

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