# Random effects in AD Model Builder

# ADMB-RE user guide

admb-project.org

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# Contents

# Chapter 1

# Introduction

This document is a user's guide to random effects modelling in AD Model Builder (ADMB). Chapter 2 is a concise introduction to ADMB, and Chapter 3 is a collection of examples selected from different fields of application. Online program code and manuals are available from the ADMB Project at admb-project.org, including

- The ADModel Builder manual
- Skaug and Fournier (2004), which describes the computational method used to handle random effect in ADMB (http://bemata.imr.no/laplace.pdf).
- The ADMB-RE example collection
- The ADMB web-forum where you can ask questions to other users (http://www.otter-rsch.ca/phpbb/).

Why use AD Model Builder for creating nonlinear random effects models? The answer consists of three words – flexibility, speed and accuracy. To illustrate these points a number of examples comparing ADMB-RE with two existing packages NLME which runs on R and Splus, and WinBUGS. In general NLME is rather fast and it is good for the problems for which it was designed, but it is quite inflexible. What is needed is a tool with at least the computational power of NLME but the flexibility to deal with arbitrary nonlinear random effects models. In section 2.2.3 we consider a thread from the R user list where a discussion about extending a model to use random effects which had a log-normal rather than normal distribution took place. This appeared to be quite difficult. With ADMB-RE this change takes one line of code. WinBUGS on the other hand is very flexible and many random effects models can be easily formulated in it. However, it can be very slow and it is necessary to adopt a

Bayesian perspective which may be a problem for some applications. A model which runs 25 times faster under ADMB than under WinBUGS may be found at: `http://otter-rsch.com/admbre/examples/logistic/logistic.html`.

## 1.1 Summary of features

**Model formulation** With ADMB you can formulate and fit a large class of nonlinear statistical models. With ADMB-RE you can include random effects in your model. Examples of such models include:

- Generalized linear mixed models (logistic and Poisson regression).
- Nonlinear mixed models (growth curve models, pharmacokinetics).
- State space models (nonlinear Kalman filter).
- Frailty models in survival analysis.
- Bayesian hierarchical models.
- General nonlinear random effects models (fisheries catch-at-age models).

You formulate the likelihood function in a template file, using a language that resembles C++. The file is compiled into an executable program (Linux or Windows). The whole C++ language is to your disposal, giving you great flexibility with respect to model formulation.

**Computational basis of ADMB-RE**

- Hyper-parameters (variance components etc.) estimated by maximum likelihood.
- Marginal likelihood evaluated by the Laplace approximation or importance sampling.
- Exact derivatives calculated using Automatic Differentiation.
- Sampling from the Bayesian posterior using MCMC (Metropolis-Hastings algorithm).
- Most features of ADMB (matrix arithmetic and standard errors, etc.) are available.

**The strengths of ADMB-RE**

- *Flexibility*: You can fit a large variety of models within a single framework.
- *Convenience*: Computational details are transparent. Your only responsibility is to formulate the loglikelihood
- *Computational efficiency*: ADMB-RE is up to 50 times faster than WinBUGS.
- *Robustness*: With exact derivatives you can fit highly nonlinear models.
- *Convergence diagnostic*: The gradient of the likelihood function provides a clear convergence diagnostic.

**Program interface**

- *Model formulation*: You fill in a C++ based template using your favorite text editor.
- *Compilation*: You turn your model into an executable program using a C++ compiler (which you need to install separately).
- *Platforms*: Windows and Linux

**How to order ADMB-RE** ADMB-RE is a module for ADMB. Both can be obtained from admb-project.org

# Chapter 2

# The language and the program

## 2.1 What is ordinary ADMB?

ADMB is a software package for doing parameter estimation in nonlinear models. It combines a flexible mathematical modelling language (built on C++) with a powerful function minimizer (based on Automatic Differentiation). The following features of ADMB make it very useful for building and fitting nonlinear models to data:

- Vector-matrix arithmetic, vectorized operations for common mathematical functions.
- Read and write vector and matrix objects to file.
- Fit the model is a stepwise manner (with 'phases'), where more and more parameters become active in the minimization.
- Calculate standard deviations of arbitrary functions of the model parameters by the 'delta method'.
- MCMC sampling around the posterior mode.

To use random effects in ADMB it is recommended that you have some experience in writing ordinary ADMB programs. In this sections we review, for the benefit of the reader without this experience, the basic constructs of ADMB.

Model fitting with ADMB has three stages: 1) Model formulation, 2) Compilation and 3) Program execution. The model fitting process is typically iterative: After having looked at the output from stage 3) one goes back to stage 1) and modifies some aspect of the program.

**Writing an ADMB program** To fit a statistical model to data we must carry out certain fundamental tasks, such as reading data from file, declaring the set of parameters that should be estimated, and finally we must give a mathematical description of the model. In ADMB you do all of this by filling in a template, which is an ordinary text file with the file-name extension '.tpl' (and hence the template file is known as the tpl-file). You therefore need a text editor, such as 'vi' under Linux or 'Notepad' under Windows, to write the tpl-file. The first tpl-file to which the reader of the ordinary ADMB manual is exposed is `simple.tpl` (listed in Section 2.2.1 below). We shall use `simple.tpl` as our generic tpl-file, and we shall see that introduction of random effects only requires small changes to the program.

A tpl-file is divided into a number of 'sections', each representing one of the fundamental tasks mentioned above. The required sections are:

| Name | Purpose |
|---|---|
| `DATA_SECTION` | Declare 'global' data objects; initialization from file |
| `PARAMETER_SECTION` | Declare independent parameters |
| `PROCEDURE_SECTION` | Specify model and objective function in C++ |

More details are given when we later look at `simple.tpl`, and a quick reference card is available in Appendix C.

**Compiling an ADMB program** After having finished writing `simple.tpl`, we want to convert it into an executable program. This is done in a DOS-window under Windows, and in an ordinary terminal window under Linux. To compile `simple.tpl`, we would under both platforms give the command:

```
$ admb -re simple
```

Here, '`$`' is the command line prompt (which may be a different symbol on your computer), and `-re` is an option telling the program `admb` that your model contains random effects. The program `admb` accepts another option `-s` which produces the 'safe' (but slower) version of the executable program. The `-s` option should be used in a debugging phase, but it should be skipped when the final production version of the program is generated.

The compilation process really consists of two steps: first `simple.tpl` is converted to a C++ program by a preprosessor called `tpl2rem` (Appendix C). An error message from `tpl2rem` consists of a single line of text, with a reference to the line in the tpl-file where the error occurs. If successful, the first compilation step results in the C++ file `simple.cpp`. In the second step `simple.cpp` is compiled and linked using an ordinary C++ compiler (which is

not part of ADMB). Error messages during this phase typically consist of long printouts, with references to line numbers in `simple.cpp`. To track down syntax errors it may occasionally be useful to look at the content of `simple.cpp`. When you understand what is wrong in `simple.cpp` you should go back and correct `simple.tpl` and re-enter the command `admb -re simple`. When all errors have been removed, the result will be an executable file, which is called `simple.exe` under Windows or `simple` under Linux.

In some situations you may want to modify the options that are passed to the C++ compiler. The script files that actually invoke the compiler reside in the `bin` directory of your ADMB installation. There are different versions of the scripts corresponding to the different combinations of command line options you can invoke `admb` with. So, given that you type `admb -re -s` the compilation script `myccsre` will be called, and subsequently the linker script `mylinksre`. By looking at the `bin` directory, or the contents of the script `admb` which also resides in this directory, you will easily figure out what is going on. (Note that older version of ADMB used slightly different naming conventions.)

**Running an ADMB-program** The executable program is run in the same window as it was compiled. Note that data are not usually part of the ADMB program (`simple.tpl`). Instead, data are being read from a file with the file name extension '.dat' (`simple.dat`). This brings us to the naming convention used by ADMB programs for input and output files: The executable automatically infers file names by adding an extension to its own name. The most important files are:

| | **File name** | **Contents** |
|---|---|---|
| Input | `simple.dat` | Data for the analysis |
| | `simple.pin` | Initial parameter values |
| Output | `simple.par` | Parameter estimates |
| | `simple.std` | Standard deviations |
| | `simple.cor` | Parameter correlations |

You can use command line options to modify the behavior of the program at runtime. The available command line options can be listed by typing:

```
$ simple -?
```

(or whatever your executable is called). The command line options that are specific to ADMB-RE are listed in Appendix 1, and are discussed in detail under the various sections. An option you probably will like to use during an experimentation phase is `-est`, which turns off calculation of standard deviations, and hence reduces the running time of the program.

**Statistical prerequisites** To use random effects in ADMB you must be familiar with the notion of a random variable, and in particular with the normal distribution. In case you are not, please consult a standard textbook in statistics. The notation $u \sim N(\mu, \sigma^2)$ is used throughout this manual, and means that $u$ has a normal (Gaussian) distribution with expectation $\mu$ and variance $\sigma^2$. The distribution placed on the random effects is called the 'prior', which is a term borrowed from Bayesian statistics.

A central concept that originates from generalized linear models is that of a linear predictor. Let $x_1, \ldots, x_p$ denote observed covariates (explanatory variables), and let $\beta_1, \ldots, \beta_p$ be the corresponding regression parameters to be estimated. Many of the examples in this manual involve a linear predictor $\eta_i = \beta_1 x_{1,i} + \cdots + \beta_p x_{p,i}$, which we also will write on vector form as $\eta = \mathbf{X}\beta$.

**Frequentist or Bayesian statistics?** A pragmatic definition of a frequentist is a person who prefers to estimate parameters by the method of maximum likelihood. Similarly, a Bayesian is a person who use MCMC techniques to generate samples from the posterior distribution (typically with noninformative priors on hyper-parameters), and from these samples generates some summary statistic such as the posterior mean. With its `-mcmc` runtime option ADMB lets you switch freely between the two worlds. The approaches complement each other rather than being competitors. A maximum likelihood fit (point estimate + covariance matrix) is a step-1 analysis. For some purposes step-1 is sufficient. In other situations, one may want to see posterior distributions for the parameters, and then the established covariance matrix (inverse Hessian of the log-likelihood) is used by ADMB to implement an efficient Metropolis-Hastings algorithm (which you invoke with `-mcmc`).

## 2.2 Why random effects?

Many people are familiar with the method of least squares for parameter estimation. Far fewer know about random effects modeling. The use of random effects requires that we adopt a statistical point of view, where the sum of squares is interpreted as being part of a likelihood function. When data are correlated, the method of least squares is sub-optimal, or even biased. But relax, random effects come to rescue!

The classical motivation of random effects is:

- To create parsimonious and interpretable correlation structures.
- To account for additional variation or overdispersion.

We shall see, however, that random effects are useful in a much wider context. For instance, the problem of testing the assumption of linearity in ordinary regression is naturally formulated within ADMB-RE (see `http://otter-rsch.com/admbre/examples/union/union.html`).

We use the `simple.tpl` example from the ordinary ADMB manual to exemplify the use of random effects. The statistical model underlying this example is the simple linear regression

$$Y_i = ax_i + b + \varepsilon_i, \qquad i = 1, \ldots, n,$$

where $Y_i$ and $x_i$ are the data, $a$ and $b$ are the unknown parameters to be estimated, and $\varepsilon_i \sim N(0, \sigma^2)$ is an error term.

Consider now the situation that we do not observe $x_i$ directly, but rather we observe

$$X_i = x_i + e_i,$$

where $e_i$ is a measurement error term. This situation frequently occurs in observational studies, and is known as the 'error in variables' problem. Assume further that $e_i \sim N(0, \sigma_e^2)$, where $\sigma_e^2$ is the measurement error variance. For reasons discussed below, we shall assume that we know the value of $\sigma_e$, so we shall pretend that $\sigma_e = 0.5$.

Because $x_i$ is not observed, we model it as a random effect with $x_i \sim N(\mu, \sigma_x^2)$. In ADMB-RE you are allowed to make such definitions through the new parameter type `random_effects_vector`. (There is also a `random_effects_matrix` which allows you to define a matrix of random effects).

1. Why do we call $x_i$ a random effect, while we do not use this term for $X_i$ and $Y_i$ (though they clearly are 'random')? The point is that $X_i$ and $Y_i$ are observed directly, while $x_i$ is not. The term 'random effect' comes from regression analysis, where it means a random regression coefficient. In a more general context 'latent random variable' is probably a better term.

2. The unknown parameters in our model are: $a$, $b$, $\mu$, $\sigma$, $\sigma_x$ and $x_1, \ldots, x_n$. We have agreed to call $x_1, \ldots, x_n$ random effects. The rest of the parameters are called hyper-parameters. Note that we place no prior distribution on the hyper-parameters.

3. Random effects are integrated out of the likelihood, while hyper-parameters are estimated by maximum likelihood . This approach is often called 'empirical Bayes', and will be considered a frequentist method by most people. There is however nothing preventing you from making it 'more Bayesian' by putting priors (penalties) on the hyper-parameters.

4. A statistician will say "this model is nothing but a bivariate Gaussian distribution for $(X, Y)$, and we don't need any random effects in this situation". This is formally true, because we could work out the covariance matrix of $(X, Y)$ by hand and fit the model using ordinary ADMB. This program would probably run much faster, but it would have taken us longer to write the code without declaring $x_i$ to be of type `random_effects_vector`. But, more important is that random effects can be used also in non-Gaussian (nonlinear) models where we are unable to derive an analytical expression for the distribution of $(X, Y)$.

5. Why didn't we try to estimate $\sigma_e$? Well, let us count the parameters in the model: $a$, $b$, $\mu$, $\sigma$, $\sigma_x$ and $\sigma_e$; totally six parameters. We know that the bivariate Gaussian distribution has only five parameters (the means of $X$ and $Y$ and three free parameters in the covariate matrix). Thus, our model is not identifiable if we also try to estimate $\sigma_e$. Instead, we pretend that we have estimated $\sigma_e$ from some external data source. This, example illustrates a general point in random effects modelling: you must be careful to make sure that the model is identifiable!

### 2.2.1 A code example

Here is the random effects version of `simple.tpl`:

```
DATA_SECTION
 init_int nobs
 init_vector Y(1,nobs)
 init_vector X(1,nobs)

PARAMETER_SECTION
 init_number a
 init_number b
 init_number mu
 vector pred_Y(1,nobs)
 init_bounded_number sigma_Y(0.000001,10)
 init_bounded_number sigma_x(0.000001,10)
 random_effects_vector x(1,nobs)
 objective_function_value f

PROCEDURE_SECTION               // This section is pure C++
 f = 0;
```

```
pred_Y=a*x+b;                    // Vectorized operations

// Prior part for random effects x
f += -nobs*log(sigma_x) - 0.5*norm2((x-mu)/sigma_x);

// Likelihood part
f += -nobs*log(sigma_Y) - 0.5*norm2((pred_Y-Y)/sigma_Y);
f += -0.5*norm2((X-x)/0.5);

f *= -1;  // ADMB does minimization!
```

**Guide for the tpl-illiterate**

1. Everything following '`//`' is a comment.

2. In the `DATA_SECTION`, variables with a `init_` in front of the data type are read from file.

3. In the `PARAMETER_SECTION`, variables with a `init_` in front of the data type are the hyper-parameters, i.e. the parameters to be estimated by maximum likelihood.

4. Variables defined in the `PARAMETER_SECTION` without the `init_` prefix can be used as ordinary programming variables under the `PROCEDURE_SECTION`. For instance, we can assign a value to the vector `pred_Y`.

5. ADMB does minimization, rather than optimization. Thus, the sign of the loglikelihood function `f` is changed in the last line of the code.

### 2.2.2 Parameter estimation

We learned above that hyper-parameters are estimated but maximum likelihood, but what if we also are interested in the value of the random effects? For this purpose ADMB-RE offers an 'empirical Bayes' approach, which involves fixing the hyper-parameters at their maximum likelihood estimates, and treating the random effects as the parameters of the model. ADMB-RE automatically calculates 'maximum posterior' estimates of the random effects for you. Estimates of both hyper-parameters and random effects are written to `simple.par`.

### 2.2.3 Log-normal random effects

Say that you doubt the distributional assumption $x_i \sim N(\mu, \sigma_x^2)$ that was made in `simple.tpl`, and that you want to check if a skewed distribution gives a better fit. You could for instance take

$$x_i = \mu + \sigma_x \exp(z_i), \qquad z_i \sim N(0,1).$$

Under this model the standard deviation of $x_i$ is proportional, but not directly equal, to $\sigma_x$. It is easy to make this modification in `simple.tpl`. In the `PARAMETER_SECTION` we replace the declaration of `x` by

```
vector x(1,nobs)
random_effects_vector z(1,nobs)
```

and in the `PROCEDURE_SECTION` we replace the prior on `x` by

```
f = - 0.5*norm2(z);
x = mu + sigma_x*exp(z);
```

This example shows one of the strengths of ADMB-RE: it is very easy to modify models. In principle you can implement any random effects model you can think of, but as we shall discuss later, there are limits to the number of random effects you can declare.

## 2.3 Random effects modeling

As with ordinary ADMB the user specifies an objective function in terms of data and parameters, but in ADMB-RE the objective function must have the interpretation as being a (negative) log-likelihood. One typically have got a hierarchical specification of the model, where at the top layer data are assumed to have a certain probability distribution conditionally on the random effects (and the hyper-parameters), and at the next level the random effects are assigned a prior distribution (typically normal). Because conditional probabilities are multiplied to yield the joint distribution of data and random effects, the objective function becomes a sum of (negative) log-likelihood contributions.

**The sign of the objective function** The reason why the objective function must hold the value of the **negative** log-likelihood is that ADMB does minimization (as opposed to maximization). In complex models, with contributions to the log-likelihood coming from a variety of data sources and random effects priors, it is recommended that you collect the contributions to the objective function using the `-=` operator of C++, i.e.

```
f -= -nobs*log(sigma_x) - 0.5*norm2((x-mu)/sigma_x);
```

In this way you avoid changing the sign of the expression for the loglikelihood expression, which makes the model/code much easier to read.

When non of the advanced features of Section 2.4 are used, you are allowed to switch the sign of the objective function at the end of the program

```
f *= -1;  // ADMB does minimization!
```

so that in fact `f` holds the value of the log-likelihood until the last line of the program.

The order in which the different loglikelihood contributions are added to the objective function does not matter, but make sure that all programming variables have got their value assigned before they enter in a prior or a likelihood expression.

In `simple.tpl` we declared $x_1, \ldots, x_n$ to be of type `random_effects_vector`. This statement tells ADMB that $x_1, \ldots, x_n$ should be treated as random effects (i.e. be the targets for the Laplace approximation), but it does not say anything about which distribution the random effects should have. In the `simple.tpl` we assumed that $x_i \sim N(\mu, \sigma_x^2)$, and (without saying it explicitly) that the $x_i$'s were statistically independent. We know that the corresponding prior contribution to the loglikelihood is

$$-n \log(\sigma_x) - \frac{1}{2\sigma_x^2} \sum_{i=1} (x_i - \mu)^2 .$$

The corresponding ADMB code is

```
f += -nobs*log(sigma_x) - 0.5*norm2((x-mu)/sigma_x);
```

Usually, the random effects will have a Gaussian distribution, but technically speaking there is nothing preventing you from replacing the above line by for instance a log-gamma density. It can be expected that the Laplace approximation will be less accurate. A change-of-variable transformation for the random

effects may be use to improve the accuracy of the Laplace approximation (not discussed in this manual).

A frequent source of error when writing ADMB-RE programs is that prior gets wrongly specified. The following trick can make the code easier to read, and has the additional advantage of being numerically stable for small values of $\sigma_x$. From basic probability theory we know that if $u \sim N(0,1)$, then $x = \sigma_x u + \mu$ will have a $N(\mu, \sigma_x^2)$ distribution. The corresponding ADMB code would be

```
f += - 0.5*norm2(u);
x = sigma_x*u + mu;
```

(This, of course, requires that we change the type of `x` from `random_effects_vector` to `vector`, and that `u` is declared as a `random_effects_vector`.) So, the trick here was to start with $N(0,1)$ distributed random effects, and to build the model from them. This is however not always the preferred strategy, as we shall see later.

Similarly, the likelihood contribution coming from data ($X_i$ and $Y_i$ in `simple.tpl`) must be added to the objective function. Typically, you will use the binomial, Poisson, gamma or Gaussian distribution for your data, but you are not restricted to these distributions. There are no built-in probability distributions, so you will have to write the mathematical expressions yourself, as we did for the Gaussian distribution above.

### 2.3.1 Correlated random effects

In some situation you will need correlated random effects, and as part of the problem you may want to estimate the elements of the covariance matrix. To ensure that the correlation matrix $C$ is positive definite, you can parameterize the problem in terms of the Cholesky factor $L$, i.e. $C = LL'$, where $L$ is a lower diagonal matrix with positive diagonal elements. There are $q(q-1)/2)$ free parameters (the non-zero elements of $L$) to be estimated, where $q$ is the dimension of $C$. Since $C$ is a correlation matrix we must ensure that its diagonal elements are unity. An example with $q = 4$ is

```
PARAMETER_SECTION
  matrix L(1,4,1,4)                  // Cholesky factor
  init_vector a(1,6)                 // Free parameters
```

```
PROCEDURE_SECTION

  int k;
  L(1,1) = 1.0;
  for(i=2;i<=4;i++)
  {
    L(i,i) = 1.0;
    for(j=1;j<=i-1;j++)
      L(i,j) = a(k++);
    L(i)(1,i) /= norm(L(i)(1,i));   // Ensures that C(i,i) = 1
  }
```

Given the Cholesky factor $L$, we can proceed in different directions. One option is to use the same transformation-of-variable technique as above: Start out with a vector $u$ of independent $N(0,1)$ distributed random effects. Then, the vector

```
x = L*u;
```

has correlation matrix $C = LL'$. To scale the variances, we multiply each component of `x` by the appropriate standard deviation.

**Large structured covariance matrices** In some situations, for instance in spatial models, $q$ will be large ($q = 100$, say). Then it is better to use the approach outlined in Section 2.5.3.

### 2.3.2 Non-Gaussian random effects

It is customary to use normally distributed random effects, but in some situations other distributions than the normal are required. The distributions currently available in ADMB-RE are: gamma, beta and robust normal distribution (mixture of 2 normal distributions). To use either of these you must

1. Define a random effect $u$ with a $N(0,1)$ distribution.

2. Transform $u$ into a new random effect $g$ using one of `something_deviate` functions described below.

In particular, to obtain av vector `g` of gamma distributed random effects (probability density $g^{a-1}\exp(-g)/\Gamma(a)$), you can use the code:

```
PARAMETER_SECTION
  init_number a            // Shape parameter
  vector g(1,n)
  random_effects_vector u(1,n,2)

PROCEDURE_SECTION
  g -= -0.5*norm2(ui);     // N(0,1) likelihood contribution from u's
  for (i=1;i<=n;i++)
    g(i) = gamma_deviate(u(i),a);
```

**Full example:** http://www.otter-rsch.com/admbre/examples/gamma/gamma.html

Similarly, to obtain beta distributed random effects (probability density proportional to $g^{a-1}(1-g)^{b-1}$) we use:

```
PROCEDURE_SECTION
  g -= -0.5*norm2(ui);    // N(0,1) likelihood contribution from u's
  for (i=1;i<=n;i++)
    g(i) = beta_deviate(u(i),a,b);
    //g(i)=beta_deviate(u(i),a,b,1.e-7);
```

The function `beta_deviate` has a fourth parameter (as in the line above that is commented out) which controls the numerical stability of the function. The use of this parameter is currently not documented.

The robust normal distribution has probability density

$$f(g) = 0.95\frac{1}{\sqrt{2\pi}}e^{-0.5g^2} + 0.05\frac{1}{c\sqrt{2\pi}}e^{-0.5(g/c)^2}$$

where $c$ is a "spread" parameter that default is set to $c = 3$. The corresponding ADMB-RE code is

```
PROCEDURE_SECTION
  g -= - 0.5*norm2(ui);    // N(0,1) likelihood contribution from u's
  for (i=1;i<=n;i++)
  {
    g(i) = robust_normal_mixture_deviate(u(i));        // c = 1.0
```

```
  //g(i) = robust_normal_mixture_deviate(u(i),2.0);  // c = 2.0
}
```

Notes about the parameters used above:

★ $a$ and $b$ are among the parameters that are being estimated, so they should have type `init_number`.

★ $c$ cannot be estimated.

It would be possible to write a version of `robust_normal_mixture_deviate` where also $c$ and the mixing proportion (fixed at 0.95 here) in this case can be estimated. The list of distribution that can be used is likely to be expanded in the future.

### 2.3.3 REML (Restricted maximum likelihood)

It is well known that maximum likelihood estimators of variance parameters can be downwards biased. The biases arises from estimation of one or more mean-related parameters. The simplest example of a REML estimator is the ordinary sample variance

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

where the devisor $(n-1)$, rather the $n$ which occurs for the maximum likelihood estimator, accounts for the fact that we have estimated a single mean parameter.

There are many ways of deriving the REML correction, but in the current context the most natural explanation is that we integrate the likelihood function (note: not the log-likelihood) with respect to the mean parameters $\beta$, say. This is achieved in ADMB-RE by defining $\beta$ as being of type `random_effects_vector`, but without specifying a distribution/prior for the parameters. It should be noted that the only thing that the `random_effects_vector` statement tells ADMB-RE is that the likelihood function should be integrated with respect to $\beta$. In linear-Gaussian models the Laplace approximation is exact, and hence this approach yields exact REML estimates. In nonlinear models the notion of REML is more difficult, but REML-like corrections are still being used.

### 2.3.4 Under the hood

The random effects are important building blocks in `simple.tpl`, but how are they treated internally in ADMB-RE? Since the random effects are not observed data they have parameter status, but we distinguish them from the hyper-parameters. This is because the $x_i$ are random variables. In the marginal likelihood function used internally by ADMB-RE to estimate hyper-parameters, the random effects are 'integrated out'. The purpose of the integration is to generate the marginal probability distribution for the observed quantities, which are $X$ and $Y$ in `simple.tpl`. In that example we could have found an analytical expression for the marginal distribution of $(X, Y)$, because only normal distributions were involved. For other distributions, such as the binomial, no simple expression for the marginal distribution exists, and hence we must rely on ADMB to do the integration. In fact, the core of what ADMB-RE does for you is that it automatically calculates the marginal likelihood, at the same time as it estimates the hyper-parameters. The integration technique used by ADMB-RE is the so-called Laplace approximation (**?**).

The algorithm used internally by ADMB-RE to estimate hyper-parameters involves iterating between the two steps:

1. The 'penalized likelihood' step: Maximizing the likelihood with respect to the random effects, while holding the value of the hyper-parameters fixed.

2. Updating the value of the hyper-parameters, using the estimates of the random effects obtained in 1).

The reason for calling the objective function in 1) a penalized likelihood, is that the prior on the random effects acts as a penalty function.

### 2.3.5 Building a random effects model that works

In all nonlinear parameter estimation problems, there are two possible explanations when your program does not produce meaningful results:

1. The underlying mathematical model is not well defined, e.g. it may be over-parameterized.

2. You have implemented the model incorrectly, e.g. you have forgotten a minus sign somewhere.

In an early phase of the code development it may not be clear which of these is causing the problem. With random effects, the two-step iteration scheme described above makes it even more difficult to find the error. We therefore advise you always to check the program on simulated data before you apply it to your real dataset. This section gives you a recipe for how to do this.

The first thing you should do after having finished the tpl-file is to check that the penalized likelihood step is working correctly. In ADMB it is very easy to switch from a random effects version of the program to a penalized likelihood version. In `simple.tpl` we would simply redefine the random effects vector `x` to be of type `init_vector`. The parameters would then be $a$, $b$, $\mu$, $\sigma$, $\sigma_x$ and $x_1, \ldots, x_n$. It is not recommended, or even possible, to estimate all of these simultaneously, so you should fix $\sigma_x$ (by giving it a phase '-1') at some reasonable value. The actual value at which you fix $\sigma_x$ is not critically important, and you could even try a range of $\sigma_x$ values. In larger models there will be more than one parameter that needs to be fixed. We recommend the following scheme:

1. Write a simulation program (in R, S-Plus, Matlab, or some other program) that generates data from the random effects model (using some reasonable values for the parameters) and writes to `simple.dat`.

2. Fit the penalized likelihood program with $\sigma_x$ (or the equivalent parameters) fixed at the value used to simulate data.

3. Compare the estimated parameters with the parameter values used to simulate data. In particular, you should plot the estimated $x_1, \ldots, x_n$ against the simulated random effects. The plotted points should centre around a straight line. If they do (to some degree of approximation) you most likely have got a correct formulation of the penalized likelihood.

If your program passes this test, you are ready to test the random effects version of the program. You redefine `x` to be of type `random_effects_vector`, free up $\sigma_x$, and apply again your program to the same simulated dataset. If the program produces meaningful estimates of the hyper-parameters, you most likely have implemented your model correctly, and you are ready to move on to your real data!

With random effects it often happens that the maximum likelihood estimate of a variance component is zero ($\sigma_x = 0$). Parameters bouncing against the boundaries usually makes one feel uncomfortable, but with random effects the interpretation of $\sigma_x = 0$ is clear and unproblematic. All it really means is that data do not support a random effect, and the natural consequence is to

remove (or inactivate) $x_1, \ldots, x_n$, together with the corresponding prior (and hence $\sigma_x$), from the model.

### 2.3.6 Linear-Gaussian random effects models

ADMB-RE was designed for non-linear random effects models. For linear-Gaussian models the likelihood is available in closed form. Also many linear models can be fitted with standard software packages. However, althougth the likelihood is explicit, it may be tedious to work out the covariance matrix of the Gaussian distribution involved. It is typically much simpler to formulate a hierarchical model with explicit latent variables. For linear-Gaussian models the Laplace approximation is exact, so ADMB-RE will produce the correct answer. An example of such a model is found at `http://otter-rsch.com/admbre/examples/bcb/bcb.html`. To make the executable program run efficiently, the command line options `-nr 1 -sparse` should be used for linear models. Also, note that REML estimates can be obtained as explained in section 2.3.3.

## 2.4 Exploiting separability

Above we have shown how to create a model containing latent random variables (random effects). This description is sufficient for models with a small number of latent random variables, but in order to deal with larger models it is necessary to exploit any special structure that the model may have. Such special structures are best described with reference to common classes of latent variable models:

- Nested random effects.
- Time series structure.
- Crossed random effects.

ADMB-RE is able to exploit these structures in two different ways, both of which help improving the performance: 1) derivative calculations can be simplifid and 2) the internal matrix computations may be performed with sparse matrix libraries. The key to achieving efficiency is to break up the computation into a series of calls to a one or more `SEPARABLE_FUNCTION`'s, in such a way that each call only involves a few latent random variables.

### 2.4.1 The first example

A simple example is the one-way variance component model

$$y_{ij} = \mu + \sigma_u u_i + \varepsilon_{ij}, \qquad i = 1, \ldots, q, \quad j = 1, \ldots, n_i$$

where $u_i \sim N(0,1)$ is a random effect and $\varepsilon_{ij} \sim N(0, \sigma^2)$ is an error term. The straightforward implementation of this model (shown only in part) is

```
PARAMETER_SECTION
  random_effects_vector u(1,q)

PROCEDURE_SECTION
  for(i=1;i<=q;i++)
  {
    g -= -0.5*square(u(i));
    for(j=1;j<=n(i);j++)
      g -= -log(sigma) - 0.5*square((y(i,j)-mu-sigma_u*u(i))/sigma);
  }
```

The efficient implementation of this model is

```
PROCEDURE_SECTION
  for(i=1;i<=q;i++)
    g_cluster(i,u(i),mu,sigma,sigma_u);

SEPARABLE_FUNCTION void g_cluster(int i, const dvariable& u,...)
  g -= -0.5*square(u);
  for(int j=1;j<=n(i);j++)
    g -= -log(sigma) - 0.5*square((y(i,j)-mu-sigma_u*u)/sigma);
```

where ... replaces the rest of the argument list (due to lack of space in this document).

It is the function call `g_cluster(i,u(i),mu,sigma,sigma_u)` that enables ADMB-RE to identify the special structure of the model, which in this case is a trivial instance of nesting. Knowing about the nesting structure enables ADMB-RE to do a series of univariate Laplace approximations, rather than a single Laplace approximation in full dimension $q$. It should then be possible

to fit models where $q$ is in the order of thousands, but this clearly depends on the complexity of the function `g_cluster`.

The following rules apply:

- ★ The argument list in the definition of the `SEPARABLE_FUNCTION` should not broken into several lines of text in the tpl-file. This is often tempting as the line typically gets long, but it results in an error message from `tpl2rem`.
- ★ Objects defined in the `PARAMETER_SECTION` must be passed as arguments to `g_cluster`. There is one exception: the objective function `g` is a global object, and does not need to be an argument. Temporary/programming variables should be defined locally within the `SEPARABLE_FUNCTION`.
- ★ Objects defined in the `DATA_SECTION` should not be passed as arguments to `g_cluster` (they are also global objects).

The data types that currently can be passed as arguments to a `SEPARABLE_FUNCTION` are:

```
int
const dvariable&
const dvar_vector&
const dvar_matrix&
```

with an example being

```
SEPARABLE_FUNCTION void f(int i, const dvariable& a, const dvar_vector& beta)
```

The qualifier `const` is required for the latter two data types, and signalizes to the C++ compiler that the value of the variable is not going to be changed by the function. You may also come across the type `const prevariable&` which means exactly the same as `const dvariable&`.

There are other rules that have to be obeyed:

- ★ No calculations involving variables defined in the `PARAMETER_SECTION` are allowed in the `PROCEDURE_SECTION`. The only use of such variables there is passing them as arguments to `SEPARABLE_FUNCTION`'s.

This rule implies that all the action has to take place inside the `SEPARABLE_FUNCTION`'s. To minimize the number of parameters that have be passed as arguments, the following programming practice is recommended when using `SEPARABLE_FUNCTION`'s:

★ The PARAMETER_SECTION should contain definitions only of the independent parameters (those variables which type has a init_ prefix) and random effects, i.e. no temporary programming variables.

All temporary variables needed for the computations should be defined locally in the SEPARABLE_FUNCTION as shown here:

```
SEPARABLE_FUNCTION void prior(const dvariable& log_s, const dvariable& u)
  dvariable sigma_u = exp(log_s);
  g -= -log_s - 0.5*square(u(i)/sigma_u);
```

### 2.4.2 Nested or clustered random effects

In the above model there is no hierarchical structure among the latent random variables (the u's). A more complicated example is provided by the following model:

$$y_{ijk} = \sigma_v v_i + \sigma_u u_{ij} + \varepsilon_{ijk}, \qquad i = 1, \ldots, q, \quad j = 1, \ldots, m, \quad k = 1, \ldots, n_{ij},$$

where the random effects $v_i$ and $u_{ij}$ are independent $N(0,1)$ distributed, and $\varepsilon_{ijk} \sim N(0, \sigma^2)$ is still the error term. One often says that the u's are nested within the v's.

Another perspective is that the data can be split into independent clusters. For $i_1 \neq i_2$ we have that $y_{i_1jk}$ and $y_{i_2jk}$ are statistically independent, so that the likelihood factors at the outer nesting level ($i$). To exploit this we use the SEPARABLE_FUNCTION as follows:

```
PARAMETER_SECTION
  random_effects_vector v(1,q)
  random_effects_matrix u(1,q,1,m)

PROCEDURE_SECTION
  for(i=1;i<=q;i++)
    g_cluster(v(i),u(i),sigma,sigma_u,sigma_v,i);
```

Note that u(i) is the i'th row of the matrix u (this is standard ADMB stuff), and it should be passed as a vector to the SEPARABLE_FUNCTION, which we would implement as follows:

```
SEPARABLE_FUNCTION void g_cluster(const dvariable& v,const dvar_vector& u,...)
  g -= -0.5*square(v);
  g -= -0.5*norm2(u);

  for(int j=1;j<=m;j++)
    for(int k=1;k<=n(i,j);k++)
      g -= -log(sigma) - 0.5*square((y(i,j,k)
                  -sigma_v*v - sigma_u*u(j))/sigma);
```

★ For a model to be detected as "clustered" each latent variable should be passed exactly once as an argument to a `SEPARABLE_FUNCTION`.

Alternative, we could have structured the program as follows:

```
PARAMETER_SECTION
  random_effects_vector v(1,q)
  random_effects_matrix u(1,q,1,m)

PROCEDURE_SECTION
  for(i=1;i<=q;i++)
    for(j=1;j<=m;j++)
      g_cluster(v(i),u(i,j),sigma,sigma_u,sigma_u,i);
```

but this would not be detected by ADMB-RE as a clustered model (because `v(i)` is passed multiple times), and hence ADMB-RE will not be able to take advantage of the fact that the likelihood factors. However, the use of the `SEPARABLE_FUNCTION` makes it possible for ADMB-RE to perform efficient calculations when invoked with the `-shess` command line option as described later.

### 2.4.3 State-space models

A simple state space model is

$$\begin{aligned} y_i &= u_i + \epsilon_i, \\ u_i &= \rho u_{i-1} + e_i, \end{aligned}$$

where $e_i \sim N(0, \sigma^2)$ is an inovation term. The log-likelihood contribution comming from the state vector $(u_1, \ldots, u_n)$ is

$$\sum_{i=2}^{n} \log\left(\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(u_i - \rho u_{i-1})^2}{2\sigma^2}\right]\right),$$

where $(u_1, \ldots, u_n)$ is the state vector. To make ADMB-RE exploit this special structure we write a `SEPARABLE_FUNCTION` named `g_conditional`, that implements the individual terms in the above sum. This function would then be invoked as follows

```
for(i=2;i<=n;i++)
  g_conditional(u(i),u(i-1),rho,sigma);
```

**Full example** http://www.otter-rsch.com/admbre/examples/polio/polio.html.

Above we have looked at a model with a univariate state vector. For multivariate state vectors, as in

$$\begin{aligned} y_i &= u_i + v_i + \epsilon_i, \\ u_i &= \rho_1 u_{i-1} + e_i, \\ v_i &= \rho_2 v_{i-1} + d_i, \end{aligned}$$

we would merge the $u$ and $v$ vectors into a single vector $(u_1, v_1, u_2, v_2, \ldots, u_n, v_n)$, and define

```
random_effects_vector u(1,m)
```

where $m = 2n$. The call to the `SEPARABLE_FUNCTION` would now look like

```
for(i=2;i<=n;i++)
 g_conditional(u(2*(i-2)+1),u(2*(i-2)+2),u(2*(i-2)+3),u(2*(i-2)+4),...);
```

where `...` denotes the arguments $\rho_1$, $\rho_2$, $\sigma_e$ and $\sigma_d$.

### 2.4.4 Crossed random effects, and more general sparse models

The simplest instance of a crossed random effects model is

$$y_k = \sigma_u u_{i(k)} + \sigma_v v_{j(k)} + \varepsilon_k, \qquad i = 1, \ldots n,$$

where $u_1, \ldots, u_N$ and $v_1, \ldots, v_M$ are random effects, and where $i(k) \in \{1, N\}$ and $j(k) \in \{1, M\}$ are index maps. The $y$'s sharing either a $u$ or a $v$ will be dependent, and in general no factoring of the likelihood will be possible. However, it is still important to exploit the fact that the $u$'s and $v$'s only enter the likelihood through pairs $(u_{i(k)}, v_{j(k)})$. Here is the code for the crossed model:

```
for (k=1;k<=n;k++)
 log_lik(k,u(i(k)),v(j(k)),mu,s,s_u,s_v);

SEPARABLE_FUNCTION void log_lik(int k, const dvariable& u,...)
 g -=  -log(s) - 0.5*square((y(k)-(mu + s_u*u + s_v*v))/s);
```

If only a small proportion of all the possible combinations of $u_i$ and $v_j$ actually occurs in the data, then the posterior covariance matrix of $(u_1, \ldots, u_N, v_1, \ldots, v_M)$ will be sparse. When an executable program produced by ADMB-RE is invoked with the `-shess` command line option, sparse matrix calculations are used. This is useful not only for crossed models. Here are a few other applications:

- For the nested random effects model as explained in section 2.4.2.
- REML estimation; recall that REML estimates are obtained by making a fixed effect random, but with no prior distribution. For the nested models in section 2.4.2, and the models with state-space structure of section 2.4.3, when using REML, ADMB-RE will to detect the cluster or time series structure of the likelihood. (This has to do with the implementation of ADMB-RE, not the model itself). However, the posterior covariance will still be sparse, and the use of `-shess` is advantageous.

### 2.4.5 Frequency weighting for multinomial likelihoods

In situations were the response variable only can take on a finite number of different values, it is possibly to reduce the computational burden enormously.

As an example, consider a situation where observation $y_i$ is binomially distributed with parameters $N = 2$ and $p_i$. Assume that

$$p_i = \frac{\exp(\mu + u_i)}{1 + \exp(\mu + u_i)},$$

where $\mu$ is a parameter and $u_i \sim N(0, \sigma^2)$ is a random effect. For independent observations $y_1, \ldots, y_n$, the loglikelihood function for the parameter $\theta = (\mu, \sigma)$ can be written:

$$l(\theta) = \sum_{i=1}^{n} \log\left[p(x_i; \theta)\right]. \tag{2.1}$$

In ADMB-RE $p(x_i; \theta)$ is approximated using the Laplace approximation. However, since $y_i$ only can take the values 0, 1 and 2, we can re-write the loglikelihood as

$$l(\theta) = \sum_{j=0}^{2} n_j \log\left[p(j; \theta)\right], \tag{2.2}$$

where $n_j$ is the number $y_i$'s being equal to $j$. Still the Laplace approximation must be used to approximate $p(j; \theta)$, but now only for $j = 0, 1, 2$, as opposed to $n$ times above. For large $n$ this can give large a large reduction in computing time.

To implement the weighted loglikelihood (2.2) we define a weight vector $(w_1, w_2, w_3) = (n_0, n_1, n_2)$. To read the weights from file, and to tell ADMB-RE that `w` is a weights vector, the following code is used:

```
DATA_SECTION
 init_vector w(1,3)

PARAMETER_SECTION
 !! set_multinomial_weights(w);
```

In addition it is necessary to explicitly multiply the likelihood contributions in (2.2) by $w$. The program must be written with `SEPARABLE_FUNCTION` as explained in Section 2.4.2. For the likelihood (2.2) the `SEPARABLE_FUNCTION` will be invoked three times.

**Full example:** http://www.otter-rsch.com/admbre/examples/weights/weights.html

## 2.5 Improving performance

In this section we discuss certain mechanisms you can use to make an ADMB-RE program run faster, or to produce more accurate estimates.

### 2.5.1 Memory management; reducing the size of temporary files

When ADMB needs more temporary storage than is available in the allocated memory buffers, it starts producing temporary files. Since writing to disk is much slower than accessing memory, it is important to reduce the size of temporary files as much as possible. There are several parameters (such as `arrmblsize`) built into ADMB that regulates how large memory buffers an ADMB program allocates at startup. With random effects the memory requirements increase dramatically, and ADMB-RE deals with this by producing (when needed) six temporary files:

| File name | Command line option |
|---|---|
| f1b2list1 | -l1 N |
| f1b2list12 | -l2 N |
| f1b2list13 | -l3 N |
| nf1b2list1 | -nl1 N |
| nf1b2list12 | -nl2 N |
| nf1b2list13 | -nl3 N |

The table also shows the command line arguments you can use to manually set the size (determined by `N`) of the different memory buffers.

When you see any of these files start growing, you should kill your application and restart it with the appropriate command line options. In addition to the options shown above there is `-ndb N` that splits the computations into N chunks. This effectively reduces the memory requirements by a factor of $N$, at the cost of a somewhat longer run time. It is necessary that $N$ is a divisor of the total number of random effects in the model, so that it is possible to split the job into $N$ iqually large parts. The `-ndb` option can be used in combination with the `-l` and `-nl` options listed above. The following rule-of-thumb for setting $N$ in `-ndb N` can be used: if there are totally $m$ random effects in the model, one should choose $N$ such that $m/N \approx 50$. For most of the models in the example collection (Chapter 3) this choice of $N$ prevents any temporary files of being created.

Consider the model `http://otter-rsch.com/admbre/examples/union/union.html` as an example. This model contains only about 60 random effects,

but does rather heavy computations with these, and as a consequence large temporary files are generated. The following command line

```
$ ./union -l1 10000000 -l2 100000000 -l3 10000000 -nl1 10000000
```

takes away the temporary files but requires 80Mb of memory. The command line

```
$ ./union -est -ndb 5 -l1 10000000
```

also runs without temporary files, requires only 20Mb of memory, but runs three times slower.

Finally, a warning about the use of these command line options. If you allocate too much memory your application will crash, and you will (should) get a meaningful error message. You should monitor the memory use of your application using "Task Manager" under Windows and the command "top" under Linux, to ensure that you do not exceed the available memory on your computer.

### 2.5.2 Limited memory Newton optimization

The penalized likelihood step (Section 2.3.4), that forms a crucial part of the algorithm used by ADMB to estimate hyper-parameters, is by default conducted using a quasi-Newton optimization algorithm. If the number of random effects is large, as it typically is for separable models, it may be more efficient to use a 'limited memory quasi-Newton' optimization algorithm. This is done using the command line argument `-ilmn N`, where `N` is the number of steps to keep. Typically `N=5` is a good choice.

### 2.5.3 Gaussian priors and quadratic penalties

In most models the prior for the random effect will be Gaussian. In some situations, such as in spatial statistics, all the individual components of the random effects vector will be jointly correlated. ADMB contains a special feature (the `normal_prior` keyword) for dealing efficiently with such models. The construct used to declaring a correlated Gaussian prior is

```
random_effects_vector u(1,n)
normal_prior S(u);
```

The first of these lines is an ordinary declaration of a random effects vector. The second line tells ADMB that `u` has a multivariate Gaussian distribution

with zero expectation and covariance matrix `S` , i.e. the probability density of **u** is

$$h(\mathbf{u}) = (2\pi)^{-1/2} \det(S)^{-1/2} \exp\left(-\frac{1}{2}\mathbf{u}' S^{-1} u\right).$$

Here, $S$ is allowed to depend on the hyper-parameters of the model. The part of the code where `S` gets assigned its value must be placed in a `SEPARABLE_FUNCTION` (see `http://otter-rsch.com/admbre/examples/spatial/spatial.html`).

★ The log-prior $\log(h(\mathbf{u}))$ is automatically subtracted from the objective function. It is thus necessary that the objective function holds the negative loglikelihood when using the `normal_prior`.

★ To verify that your model really is partially separable you should try replacing the `SEPARABLE_FUNCTION` keyword with an ordinary `FUNCTION`. Then verify on a small subset of your data that the two versions of the program produce the same results. You should be able to observe that the `SEPARABLE_FUNCTION`-version runs faster.

### 2.5.4 Importance sampling

The Laplace approximation may be inaccurate in some situations . The quality of the approximation may then be improved by adding an importance sampling step. This is done in ADMB-RE by using the command line argument `-is N seed`, where `N` is the sample size in the importance sampling and `seed` (optional) is used to initialize the random number generator. Increasing `N` will give better accuracy, at the cost of a longer run time. As a rule-of-thumb you should start with `N=100`, and increase `N` stepwise by a factor of 2 until the parameter estimates stabilize.

By running the model with different seeds you can check the Monte Carlo error in your estimates, and possibly average across the different runs to decrease the Monte Carlo error. Replaing the `-is N seed` option with a `-isb N seed` gives you a "balanced" sample, which in general should reduce the Monte Carlo error.

For large values of `N`, the option `-is N seed` will require a lot of memory, and you will see that huge temporary files are produced during the execution of the program. The option `-isf 5` will split the calculations relating to importance sampling into 5 (or any number you like) batches. In combination with the techniques discussed in Section 2.5.1, this should reduce the storage requirements. An example of a command line is:

```
lessafre -isb 1000 9811 -isf 20 -cbs 50000000 -gdb 50000000
```

The `-is` option can also be used as a diagnostic tool for checking the accuracy of the Laplace approximation. If you add the `-pis` (print importance sampling) the importance sampling weights will be printed at the end of the optimization process. If these weights do not vary much, the Laplace approximation is probably doing well. On the other hand, if a single weight dominates the others by several orders of magnitude, you are in trouble, and it is likely that even `-is N` with a large value of `N` is not going to help you out. In such situations, reformulating the model, with the aim of making the loglikelihood closer to a quadratic function in the random effects, is the way to go. See also the following section.

### 2.5.5 Gauss-Hermite quadrature

In the situation where the model is separable of type "block diagonal Hessian" with only a single random effect in each block (see Section 2.4), Gauss-Hermite quadrature is available as an option to the Laplace approximation and the `-is` option (importance sampling). It is invoked with command line option `-gh N` where `N` is the number of quadrature points.

### 2.5.6 Phases

A very useful feature of ADMB is that it allows the model to be fit in different phases. In the first phase you estimate only a subset of the parameters, with the remaining parameters being fixed at their initial values. In the second phase more parameters are turned on, and so it goes. The phase in which a parameter becomes active is specified in the declaration of the parameter. By default a parameter has phase 1. A simple example would be

```
PARAMETER_SECTION
  init_number a(1)
  random_effects_vector b(1,10,2)
```

where `a` becomes active in phase 1, while `b` is a vector of length 10 that becomes active in phase 2. With random effects we have the following rule-of-thumb for the use of phases:

1. Activate the random effects and the corresponding variance parameter in phase 2.

2. Activate the remaining hyper-parameters in phase 1.

When there are more than one random effects vector, it may be advantageous to let these become active in different phases.

During program development it is often useful to be able to completely switch a parameters off. A parameter is inactivated when given phase '-1' as in

```
PARAMETER_SECTION
  init_number c(-1)
```

The parameter is still part of the program, and its value will still be read from the pin-file, but it does not take part in the optimization (in any phase).

For further details about phases, please consult the section 'Carrying out the minimization in a number of phases' in the ADMB manual (not this document).

### 2.5.7 MCMC

There are two different MCMC methods built into ADMB-RE: `-mcmc` and `-mcmc2`. Both are based on the Metropolis-Hastings algorithm. The former generates a Markov chain on the hyper-parameters only, while `-mcmc2` generates a chain on the joint vector of hyper-parameters and random effects. (Some sort of rejection sampling could be used with `-mcmc` to generate values also for the random effects, but this is currently not implemented). The advantages of `-mcmc` are:

- Because there typically is a small number of hyper-parameters, but a large number of random effects, it is much easier to judge convergence of the chain generated by `-mcmc` than that generated by `-mcmc2`.
- The `-mcmc` chain mixes faster than the `-mcmc2` chain.

The disadvantage of the `-mcmc` option is that it is slow, because it relies on evaluation of the marginal likelihood by the Laplace approximation. It is recommended to run (separately) both of `-mcmc` and `-mcmc2` to verify that they yield the same posterior for the hyper-parameters.

## 2.6 Are all the ADMB-functions in ADMB-RE?

You will find that not all the functionality of ordinary ADMB has yet been implemented in ADMB-RE. Functions are being added all the time.

# Appendix A

# Command line options

A list of command line options accepted by ADMB programs can be obtained by giving the option `-?` to the application, for instance `simple -?`. The following command line options are specific to ADMB-RE. Please consult the ordinary ADMB manual for the rest of the command line options.

| Option | Explanation |
|---|---|
| `-is N seed` | use importance sampling with sample size `N` and `seed` |
| `-pis` | print importance sampling weights |
| `-ilmn N` | `N`-step limited memory quasi Newton for random effects |
| `-gh N` | perform `N` point Gauss-Hermite quadrature |
| `-nr N` | perform `N` Newton-Raphson steps in the Laplace approximation |
| `-imaxfn N` | perform `N` optimization steps in the Laplace approximation |
| `-shess` | invoke sparse matrix libraries |
| `-noinit` | do not initialize random effects before inner optimzation |
| `-ndb N` | splits computations into N chunks |
| `-l1 N` | set the size of buffer `f1b2list1` to `N` |
| `-l2 N` | set the size of buffer `f1b2list12` to `N` |
| `-l3 N` | set the size of buffer `f1b2list13` to `N` |
| `-nl1 N` | set the size of buffer `nf1b2list1` to `N` |
| `-nl2 N` | set the size of buffer `nf1b2list12` to `N` |
| `-nl3 N` | set the size of buffer `nf1b2list13` to `N` |

# Appendix B

# Interfacing ADMB with R

R is a popular freely available software package for statistical analysis. It is convenient to be able to call ADMB programs from R. This appendix explains how to:

- Write data to the `.dat` and `.pin` files.
- Call an exe-file produced with ADMB (via the `system()` function in R).
- Read back the `.par` and `.std` files.

It is also possible to compile an ADMB program into an dll that can be linked with R, as described in the chapter "Creating Dynamic Link Libraries with AD Model Builder" of the ADMB manual.

Consider the simple linear regression ($y$ against $x$). We first generate data in R

```
> y = rnorm(3)
> x = rnorm(3)
> dat_write("simple",list(n=length(y),y=y,x=x))
```

which produces the file `simple.dat`:

```
# "simple.dat" produced by dat_write() from ADMButils; Wed ...
# n
 3

# y
```

```
 0.4157458 0.07686372 -0.709638

# x
 -1.662676 1.193920 -0.08753698
```

Currently, `dat_write()` handles vector and matrix arguments, but not 3-dimensional arrays. Similarly, `pin_write()` writes initial values for the parameters to `simple.pin`.

To invoke `simple.exe` (assumed to exists in the directory where R is running) we give the command:

```
> system("simple",T)
```

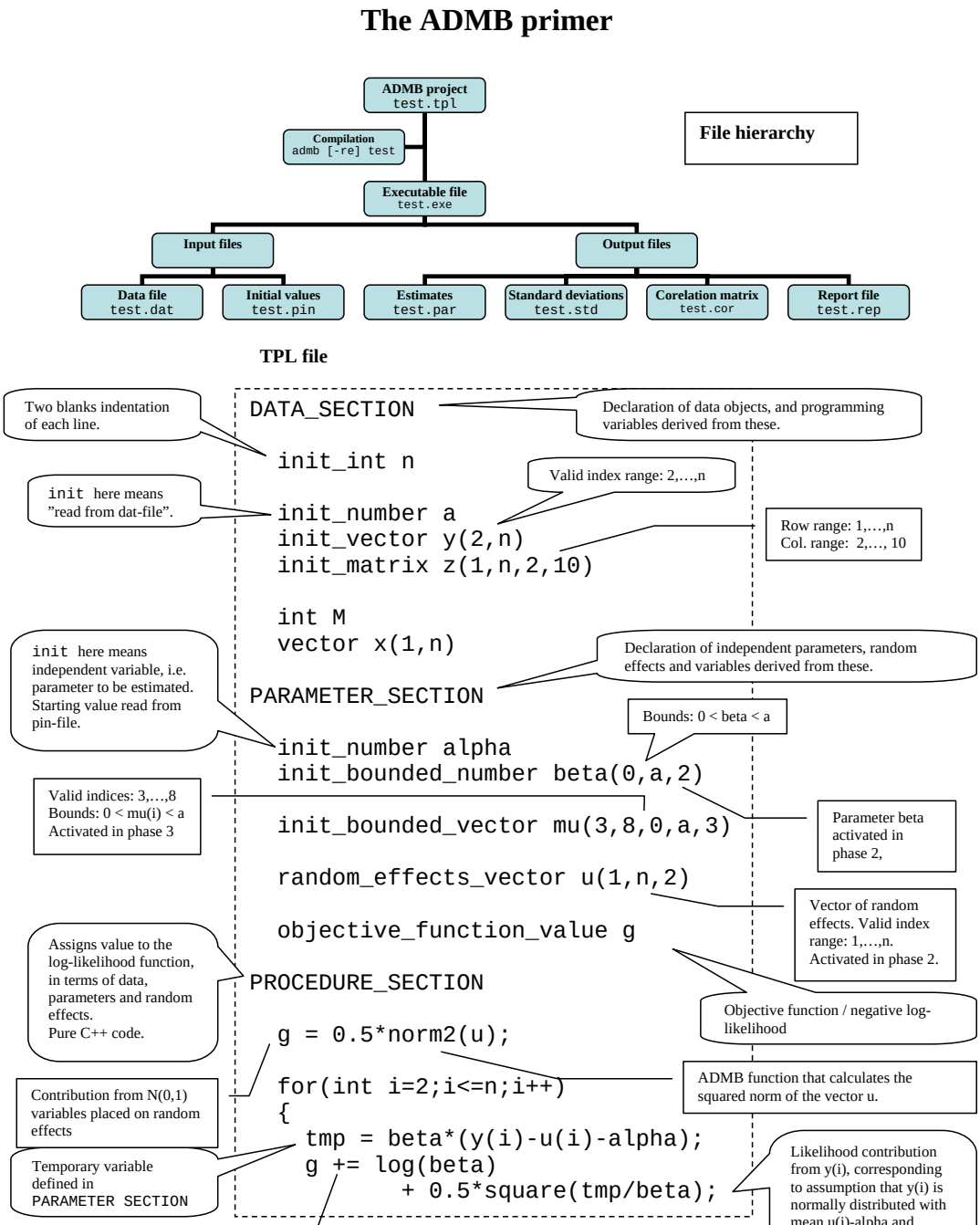
We then read back the results using either of the commands

```
> L1 = par_read("simple")
> L2 = std_read("simple")
```

which both return list objects (`L1` and `L2`).

# Appendix C

# Quick references



# Compiling ADMB programs

To compile `model.tpl` in a DOS/Linux terminal window:

```
admb [-s] [-re] model
```

where the options
`-s` yields the ”safe” version of the exe-file
`-re` yis used to invoke the random effect module

Two stages of compilation:

- Preprosessor: `tpl2cpp` or `tpl2rem`
- C++ compiler (Borland, Visual C++, etc.)