

# ASReml Update

What's new in Release 4.1

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Arthur Gilmour acknowledges the grace of God through Jesus Christ who enables this research to proceed. Be exalted O God, above the heavens: and Thy glory above all the earth. Psalm 108:5.

# <span id="page-2-0"></span>Preface

### Developments in ASReml Release 4

There are a number of new developments in Release 4. These are described in Chapter [1.](#page-8-0) Developments associated with input include generating initial values, generating a template to allow an alternative way of presenting parametric information associated with variance structures, new facilities for reading in data files and defining factor names and improved facilities for reading relationship matrices. Among the developments associated with analysis are making it easier to specify functions of variance parameters using names rather than numbers, fitting factor effects with large random regression models, such as commonly used with marker data, fitting linear relationships among variance structure parameters and calculating information criteria. The developments associated with output include writing out design matrices.

#### New model specification using a functional approach

The main development in ASReml Release 4 is a new model specification using a functional approach. Prior to Release 4 a structural specification was used in which variance models were applied by imposing variance structures on random model terms and/or the residual error term after the mixed model had been specified. In this case, the variance models were presented in a separate part of the input file. The functional specification offers a simpler alternative to the structural specification in which the variance structures for random model terms and the residual error term are specified in the linear mixed model definition by wrapping terms with the required variance model function. This functional approach is more concise, less error-prone and more automatic for specifying multi-section residual variances.

The functional model specification has been developed from the model implementation of ASReml-R and offers a more seamless movement between platforms. A complete discussion of the functional specification, with reference to the structural specification, is presented in Chapter [2.](#page-30-0) Chapter [3](#page-69-0) takes examples from the User Guide and compares the functional and structural specifications.

## Who should read this document?

This document is for existing users who wish to keep abreast of the developments with Release 4. Chapter [2](#page-30-0) is primarily for existing users who wish to migrate to the functional model specification. Users who are new to ASReml with Release 4 are referred to the ASReml User Guide for this version.

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# <span id="page-8-0"></span>1 Developments in ASReml Release 4

This chapter is a summary of the developments in Release 4 associated with

- input (Section [1.1\)](#page-8-1) including the generation of initial values, the generation of a template to allow an alternative way of presenting parametric information associated with variance structures and improved facilities for reading relationship matrices
- analysis (Section [1.2\)](#page-14-2) including making it easier to specify functions of variance parameters using names rather than numbers, fitting factor effects with large random regression models,such as commonly used with marker data, fitting linear relationships among variance structure parameters and calculating information criteria
- **output** (Section [1.3\)](#page-27-0) including writing out design matrices.

Another development is the implementation of an alternative way of specifying the mixed model. The distinguishing feature of this specification is that the variance models for individual terms are specified by applying variance model functions to the terms in the model definition line(s). This is in contrast to the structural specification of versions prior to Release 4 in which the variance models were only imposed after the mixed model definition line(s). Some users might find this functional specification more natural and less error prone. There is a comprehensive discussion of the specification in Chapter [2](#page-30-0) and Chapter [3](#page-69-0) compares the structural and functional specifications for a range of User Guide examples.

## <span id="page-8-2"></span><span id="page-8-1"></span>1.1 Improvements to input

#### 1.1.1 Generating initial values for variance structure parameters

In ASReml 3 it was necessary to supply initial values for variance structure parameters except for the default variance structure for a random model term, where the default initial variance (ratio) parameter value was 0.1. In ASReml 4, it is not generally necessary to supply initial values. In this release, if the user uses \* instead of the initial value(s) then ASReml provides initial values for variance structure parameters based on knowledge of the phenotypic variance of the response. Occasionally these initial values are not adequate and more appropriate values will need to be supplied by the user, perhaps using prior information <span id="page-9-0"></span>or results from a simplified analysis.

## 1.1.2 Using templates to set parametric information associated with variance structures using .tsv and .msv files

ASReml 3 needed initial values for most variance structure parameters and allowed specification of parametric constraints and relationships (equality and scale) between parameters to be defined. This parametric information was interspersed within the structure definition. Release 4 allows an alternative way of specifying this parametric information, essentially constructing a table in a .tsv file, with the rows labelled by the specific parameters, columns for initial values and parametric constraints, and two columns that allow specification of relationships. This .tsv file is written by ASReml after the input file has been parsed; using \* to represent initial values and setting !MAXITER 0 for an easy construction.Once the .tsv file has been edited it can be read by inserting !TSV on the data file line. As an example

```
Wolfinger Rat data
treat !A
wt0 wt1 wt2 wt3 wt4
subject * !=V0
wolfrat.dat !skip 1 !ASUV !MAXITER 0
wt0 wt1 wt2 wt3 wt4 Trait treat Trait.treat
1 \t2 \t027 0 ID #error variance
Trait 0 US * #* indicates generates initial values
generates a .tsv file.
# This .tsv file is a mechanism for resetting initial parameter values
# by changing the values here and rerunning the job with !TSV
# You may only change values in the last 4 fields.
# Fields are:
# GN, Term, Type, PSpace, Initial_value, RP_GN, RP_scale.
5, "units.us(Trait);us(Trait) 1", G, P, 4.7911110 , 5, 1
6, "units.us(Trait);us(Trait) 2", G, P, 5.0231481 , 6, 1
7, "units.us(Trait);us(Trait) 3", G, P, 15.298889 , 7, 1
8, "units.us(Trait);us(Trait)_4", G, P, 4.8438271, 8, 1
9, "units.us(Trait);us(Trait) 5", G, P, 11.264815, 9, 1
10, "units.us(Trait);us(Trait) 6", G, P, 26.095692 , 10, 1
11, "units.us(Trait);us(Trait) 7", G, P, 4.6882715 , 11, 1
12, "units.us(Trait);us(Trait) 8", G, P, 10.824074 , 12, 1
13, "units.us(Trait);us(Trait) 9", G, P, 27.332887 , 13, 1
14, "units.us(Trait);us(Trait) 10", G, P, 71.875403 , 14, 1
15, "units.us(Trait);us(Trait) 11", G, P, 3.9083333 , 15, 1
16, "units.us(Trait);us(Trait) 12", G, P, 10.292592 , 16, 1
```

```
17, "units.us(Trait);us(Trait) 13", G, P, 34.137962 , 17, 1
18, "units.us(Trait);us(Trait) 14", G, P, 69.287036 , 18, 1
19, "units.us(Trait);us(Trait) 15", G, P, 141.97296 , 19, 1
```
Parameter constraints and initial values can be changed by editing the values in the PSpace and Initial value columns. Scale relationships can be introduced by noting that the full set of parameters can be related to a subset of parameters and scale factors such as

 $parameter = subset parameter * scale$ 

or

```
GN column parameter, RP_GN column parameter * RP_scale value
```
where GN, RP\_GN and RP\_scale are columns in the .tsv file. The relationships generated by

```
VCC 2
5 6 8 11 15 7 * 2 9 * 2 12 * 2 16 * 2 #parameters 6 8 11 15 are equal to 5
#7 9 12 16 are twice 5
10 13 17 #parameters 13 and 17 are equal to 10
#the full set of parameters 5-19 can therefore be expressed in terms of the subset parameters
5, 10 ,14, 18 and 19
```
can be introduced by editing the RN GN and RP scale columns. Some users would prefer to insert initial values into this .tsv file under the Initial value column. As an example, the file below contains values based on using 4.8, 26, 70, 35 and 70 for parameters 5, 10, 14, 18 and 19. The data values in the .tsv file become

```
# GN, Term, Type, PSpace, Initial_value, RP_GN, RP_scale.
5, "units.us(Trait);us(Trait) 1", G, P, 4.8 , 5, 1.0000
6, "units.us(Trait);us(Trait) 2", G, P, 4.8 , 5, 1.0000
7, "units.us(Trait);us(Trait) 3", G, P, 9.6 , 5, 2.0000
8, "units.us(Trait);us(Trait) 4", G, P, 4.8 , 5, 1.0000
9, "units.us(Trait);us(Trait)_5", G, P, 9.6, 5, 2.0000
10, "units.us(Trait);us(Trait) 6", G, P, 26 ,10, 1.0000
11, "units.us(Trait);us(Trait) 7", G, P, 4.8 , 5, 1.0000
12, "units.us(Trait);us(Trait) 8", G, P, 9.6 , 5, 2.0000
13, "units.us(Trait);us(Trait) 9", G, P, 26 , 10, 1.0000
14, "units.us(Trait);us(Trait) 10", G, P, 70 , 14, 1.0000
15, "units.us(Trait);us(Trait) 11", G, P, 4.8 , 5, 1.0000
16, "units.us(Trait);us(Trait) 12", G, P, 9.6 , 5, 2.0000
17, "units.us(Trait);us(Trait) 13", G, P, 26 , 10, 1.0000
18, "units.us(Trait);us(Trait) 14", G, P, 35 , 18, 1.0000
19, "units.us(Trait);us(Trait) 15", G, P, 70 , 19, 1.0000
```
Sometimes users wish to rerun a job making changes to the final values, parametric constraints and relationships (equality and scale) between parameters. A file .msv is produced, similar to .tsv but containing final values that can be edited and used with !MSV. If !TSV

(or !MSV) is specified ASReml will read the current (created with the same PART number) .tsv (or .msv) file. If there is no current .tsv (or .msv file), a non-current (produced from a different PART of the same job) .tsv (or .msv) file will be read.

Alternative ways of specifying !TSV and !MSV are !CONTINUE 2 and !CONTINUE 3 and these qualifiers can be used as options on the command line as -C2 and -C3. Note that the constraints in the .tsv/.msv files take precedence over those in the .as file.

If f=filename, with no extension, is used with !CONTINUE, !TSV or !MSV, ASReml will use the file f.rsv, f.tsv or f.msv. If  $f=f$ ilename.xsv with  $x=r$ , t or m is used with !CONTINUE, !TSV or !MSV, ASReml will use the file f.xsv. If the specified file is not present, ASReml reverts to reading the previous .rsv file.

## <span id="page-11-0"></span>1.1.3 Skipping fields during data input

The meaning of the  $\mathsf{ISKIP}$  n qualifier differs with context. It is most commonly specified after the name of a pedigree or data file to instruct ASReml to ignore the first n lines of the file (presumably heading lines). !SKIP can also be used to skip columns when reading in a data file. For example,

#### A !SKIP 1 B

instructs ASReml to skip 1 data field before reading the field to be labelled A.

A new qualifier, !CSKIP c, is now available to skip data fields (columns) when reading the data. It is an alternative to  $\mathsf{ISKIP}\ n$  but is more logically placed. For example,

#### !CSKIP 1 A B

does the same as the above !SKIP command, that is, skips the first data field and reads the second and third data fields into variables A and B. Likewise,

#### !CSKIP n A B

skips the first n data fields and reads the next two fields into variables A and B.

<span id="page-11-1"></span>We suggest using !CSKIP in preference to !SKIP for skipping data fields.

## 1.1.4 Setting the order of alphanumeric factor levels

An !L qualifier associated with the !A qualifier was available in Release 3 and pre-declared the levels of alphanumeric factors and their order. ASReml will now accept a filename argument where the first field of each line of the file contains the names of the levels. If the filename has Identity as the first name on the first line, the first line is ignored. The # character is treated as the beginning of a comment; the # itself and the following characters are ignored, as are blank lines. Consequently, a level label may not contain the character #. If the filename includes embedded blanks, or has no file extension, it must be enclosed in quotes:

```
Genotype !A !L MyNames.txt
Genotype !A !L 'My Names.txt'
Genotype !A !L 'MyNames'
```
When actually reading the data, any label that is not already defined is appended to the list when it is encountered. One use of this qualifier is to ensure that the data is coded according to the order of the identities (ID's) used when forming .grm or .giv files; supplying the order in a text file. For example, if the file Idnames.txt contains the list and has 1 header line, define ID as

ID !A 450 !L Idnames.txt !SKIP 1

where 450 is the number of levels. Note that in this context of defining a label file, ASReml interprets !SKIP as skipping a line rather than a column (field) in the names file. Refer to the User Guide for information on data file types.

## <span id="page-12-0"></span>1.1.5 Extra facilities for reading relationship matrix (including GRM) files

#### New model names

In previous releases of ASReml, a pedigree file could be associated with a factor, and a numerator relationship matrix was generated and could be used as a variance structure. Slightly illogically, this structure was specified in models using AINV (Additive Inverse Matrix). Similarly, generalised relationship matrices (grm) or their inverses (giv) could be read in and giv() and GIV could be used in the model specification. In Release 4, ASReml allows the use of NRM as a synonym for AINV and the use of  $nrm(f)$  on the model line. Furthermore, GRMn and grmn(f) can be used as synonyms for GIVn and  $giv(f,n)$  respectively, where f is the model term variable to which the structure is applied and  $n$  is the ordinal number of the GIV/GRM matrix being associated with f.

#### GRM files

GRM and GIV files will be read assuming single/double precision lower triangle row-wise binary format if the file extension is .sgiv, .dgiv, .sgrm or .dgrm.

!PRECISION n changes the value used to declare a singularity when inverting a GRM file from 1D-7 to 1D-n.

!SAVEGIV on the GRM line has been extended to

!SAVEGIV 3 which writes the GIV matrix as an .sgiv file, or

!SAVEGIV 4 which writes the GIV matrix as a .dgiv file, where .sgiv is single precision lower triangle row-wise binary and .dgiv is double precision lower triangle row-wise binary.

Diagnostics when processing GRM files have been improved. ASReml now tests the GRM matrix and reports if it is not positive definite. In this case, 3 qualifiers may be used to

#### 1.1 Improvements to input

allow ASReml to proceed. If the matrix has positive and negative eigenvalues, !ND instructs ASReml to ignore the condition and proceed anyway. If the matrix is positive semi-definite (positive and zero eigenvalues), !PSD allows ASReml to introduce Lagrangian multipliers to accommodate linear dependencies and rows with zero elements, and allows ASReml to proceed. Linear dependencies occur, for example, when the list of individuals includes clones. Rows with zero elements occur when the GRM represents a dominance matrix, and the list of individuals includes fully inbred individuals which, by definition, have zero dominance variance. If the matrix has positive, zero and negative eigenvalues, !NSD may be used to allow ASReml to continue. The zero eigenvalues are handled as for !PSD.

Another example of !L (Section [1.1.4\)](#page-11-1) is in analysis on data with 2 relationship matrices based on two separate pedigrees. ASReml only allows one pedigree file to be specified but can create an inverse relationship matrix and store the result in a GIV file. So, 2 relationship matrices based on two separate pedigrees may be used by generating a GIV file from one pedigree and then using that GIV file and the other pedigree in a subsequent run. To process the GIV file properly, we must also generate a file with identities as required for the GIV matrix. An example of this is if the file Hybrid.as includes

```
!PART 1
Mline !P
Fline !A
...
Mline.ped !GIV !DIAG #!GIV generates the file Hybrid1A.giv and !DIAG
#generates Hybrid1.aif which contains the identifier names
!PART 2 #reads in inverse additive relationship matrix generated in !PART 1
Mline !A !L Hybrid1.aif !SKIP 1#associates identifier names with levels of Mline
#used in giv file
Fline !P
...
Fline.ped !GIV !DIAG
Hybrid1 A.giv #formed in part 1 from Mline.ped
Hybrid.asd !SKIP 1
...
... grm1(Mline) nrm(Fline) #using new synonyms and functions
```
### <span id="page-13-0"></span>1.1.6 Handling the  $#$  character in data files

The general (data line) qualifier !SPECIALCHAR causes  $\#$  to be treated as an ordinary character in the data file, rather than to have its usual meaning, that is, to ignore the rest of the *input line.* ASReml generates a warning message when the  $\#$  character appears in the data file and !SPECIALCHAR has not been used.

## <span id="page-14-0"></span>1.1.7 Extension to the ! FILTER qualifier

The !FILTER f qualifier is used with the !SELECT s qualifier to select only the data records that have the value s in field f. This has been extended by addition of the qualifier !EXCLUDE  $e$  to ignore all data records that do have the value  $e$  in field  $f$ .

## <span id="page-14-1"></span>1.1.8 Using binary MBF files

The !MBF statement extracts covariate values corresponding to levels of a factor from an auxiliary file. This file may now be a binary format file, with file extension .bin indicating 32bit real binary numbers and .dbl indicating 64bit real binary values. Files with these formats can be easily created in a preliminary run using the !SAVE qualifier. The advantage of using a binary file is that reading the file is much quicker. This is important if the file has many fields and is being accessed repeatedly, for example

```
!CYCLE 1:1000
!MBF mbf(Geno) markers.dbl !key 1 !RFIELD $I !rename M$I
... !r M$I
```
## <span id="page-14-3"></span><span id="page-14-2"></span>1.2 Improvements to analysis

### 1.2.1 Fitting linear relationships among variance structure parameters

The user may wish to define relationships between particular variance parameters. For example, consider an experiment in which two or more separate trials are sown adjacent to one another at the same trial site, with trials sharing a common plot boundary. In this case it might be sensible to fit the same spatial parameters and error variances for each trial. In other situations it can be sensible to define the same variance structure over several model terms. ASReml 3 catered for equality and multiplicative relationships among variance parameters. In ASReml 4 linear relationships among variance structure parameters can be defined through a simple linear model and by supplying a design matrix for a set of parameters. The design matrix is supplied as an ascii file containing a row for each parameter in a set of contiguous parameters and a column for each new parameter. This design matrix is associated with the job through a statement after the residual model definition line(s), of the form:

#### VCM first [intermediate] last new filename

where *first* is the parameter number of the first parameter in the set, *intermediate* is required unless all the intermediate parameters are involved, last is the parameter number of the last parameter in the set, new is the number of new parameters filename is the name of the file containing the design matrix.

For example, the Wolfinger rats example involves modelling a  $5\times 5$  symmetric residual matrix. Wolfinger Rat data

treat !A

```
wt0 wt1 wt2 wt3 wt4
subject * !=V0
wolfrat.dat !skip 1
wt0 wt1 wt2 wt3 wt4 ∼ Trait treat Trait.treat
1 2 0
27 0 ID #error variance
Trait 0 US * #* indicates generates initial values
#uses 15 parameters numbered 5-19 generating symmetric matrix
#5
#6 7
#8 9 10
#11 12 13 14
#15 16 17 18 19
```
[Wolfinger](#page-89-1) [\(1996\)](#page-89-1) reports the fitting of the HuynhFeldt variance structure to this data. This structure is of the form

$$
\begin{array}{rcl}\n\boldsymbol{\sigma}_{ii} & = & \boldsymbol{\sigma}_{ni} \\
\boldsymbol{\sigma}_{ij} & = & 1/2 \left( \boldsymbol{\sigma}_{ni} + \boldsymbol{\sigma}_{nj} \right) - \boldsymbol{\sigma}_{no} \quad j < i \leq p\n\end{array}
$$

In the rats example, the relationship between the original and new parameters is  $\sigma = M \sigma_n$ where  $\sigma$  and  $\sigma_n$  are  $15 \times 1$  and  $6 \times 1$  vectors respectively, and M is a  $15 \times 6$  matrix:



A way of fitting this model would be to put the matrix values in a file HuynhFeldt.vcm and replace the G Trait specification by

```
Trait 0 US !GU
45 20 45 20 20 45 20 20 20 45 20 20 20 20 45
#Supply start values because raw SSP generates bad initial values
#for HuynhFeldt structure because it does not fit well
```
#### VCM 5 19 6 HuynhFeldt.vcm #parameters 5 to 19 explained in terms of 6 parameters

Note that if the user fits another model with differing numbers of variance structure parameters so that the variance structure parameters are renumbered, then all the user needs to do to continue with the same relationships is to change the first and last parameters on the VCM line.

<span id="page-16-0"></span>Important The VCM statement must be placed after any residual definition line(s).

## 1.2.2 Data order, filling in the spatial grid

In Release 3, the qualifiers !SECTION, !ROWFACTOR and !COLUMNFACTOR in combination with an appropriate *Variance header line*, generated an  $AR1\times ARI$  variance structure for each section. That is, it created the internal structures to fit this model and wrote the lines which specified this structure to the .res so that they could be pasted into a revised .as file.

However, to fit this model, it is necessary that the complete grid of plots be represented in the data file, even though some of them may be missing a yield response. In ASReml 4, if these qualifiers are specified and the model term mv is fitted, ASReml will sort the data on the three fields specified and insert 'missing value' records to complete the row/column grid for each section.

## <span id="page-16-1"></span>1.2.3 Information criteria

For comparing nested models we recommend the REML likelihood ratio test (REMLRT), see Section 2.5 of the User Guide. The Akaike Information Criterion (AIC) and the Bayesian Information Criterion (BIC) are defined in equation 2.15 of the User Guide. The AIC and BIC are provided for the convenience of users but without any formal recommendation for their use. The number of parameters includes the number of linear parameters estimated and the number of variance structure parameters estimated, excluding variance parameters fixed at a boundary during the estimation procedure. The value used in calculating AIC and BIC is reported, giving the opportunity for the user to verify/modify this number.

All of these statistics are based on the REML log-likelihood statistics and are only valid if the fixed effects model is unchanged between runs and is fitted in the same order (ie. the same effects are aliased in the case where the model is over-parameterized).

## <span id="page-16-2"></span>1.2.4 Conditional coding

The facilities for manipulating job coding have been extended with the high level qualifiers in Table [1.1.](#page-17-1) These are high level in the sense that they can appear at any point in the command file, provided the result can be formed at that point.

### <span id="page-17-0"></span>1.2.5 Processing random terms as DENSE

ASReml uses link list matrix methods for the sparse equations and has always included random model terms in these sparse equations. However, in the case of GRM matrices, they are typically quite large (several thousand) and dense, and it would be more efficient generally to process them as such. Release 4 has a !GDENSE qualifier (set just before the model line). If !GDENSE is set and the first random term is a GRM term, its equations will be processed as DENSE. For an example with 3226 rows in the GRM matrix, !GDENSE reduced the iteration time from 196 to 175 seconds.

Table 1.1: High level qualifiers

<span id="page-17-1"></span>

## 1.2 Improvements to analysis



## High level qualifiers

## <span id="page-19-0"></span>1.2.6 Factor effects with large Random Regression models

One use of the GRM matrix is to allow more computationally efficient fitting of random regression models associating  $u$ , a vector of f factor effects with  $v$  a vector of m regression effects through the model  $u = M v$  where the matrix M contains m regressor variables for each of the  $f$  levels of the factor. Direct fitting of the regression effects is facilitated by using the my basis function (mbf function) associating the regressor variables to the levels of the factor, essentially fitting  $ZMv$  where Z is the design matrix linking observations to the levels of the factor. But if m is much bigger than  $f$ , it is more computational efficient to fit an equivalent model  $\boldsymbol{Z}\boldsymbol{u}$  with a variance structure for  $\boldsymbol{u}$  based on  $\boldsymbol{M}\boldsymbol{M}'$ . ASReml can read the matrix  $M$  associated with a factor and group of regressor variables from a .gr file, construct a GRM matrix  $(G = MM'/s$  with s a scale parameter), fit the equivalent model and report both factor and regressor predictions. One common case of this model is when  $\boldsymbol{u}$  represents genotype effects, the regressors represent SNP marker counts (typically  $0/1/2$ representing allelle counts and 0 and 2 representing homozygotes) and  $\boldsymbol{v}$  are marker effects.

The .grr file is specified after any pedigree file and before the data file (with any other GRM files). There may only be one .grr file. It is assumed to contain a row for each level of the factor, each row containing m regressor values. Optionally the factor level name associated with the i-th row can be included before the relevant regressor values. Also a heading row might include a name for each field/regressor variable. Superfluous fields before the factor or regressor fields can be skipped and superfluous rows before the regressor information can be skipped.

The syntax for specifying and reading the .grr file is

M.grr [!CSKIP  $c_1$ ] Factor [f] [!NOID] [!CSKIP  $c_2$ ] Regressors [m] [!NONAMES] [!SKIP s] where

M.grr is the name of the file to be read, !CSKIP  $c_1$  indicates  $c_1$  fields are to be skipped before the factor identifiers are read,

Factor is the name of the variable in the data that is associated with the regressors,

f sets the maximum number of levels (default 1000) of Factor with regressor data; ASReml will count the actual number,

!NOID indicates that the factor identifiers are not present in the .grr file,

!CSKIP  $c_2$  indicates  $c_2$  fields are to be skipped before the regressor variables are read,

Regressors is the name for the set of regressor variables,

m sets the number of regressor variables (default is the number of names found); must be set if there are extraneous fields to be ignored,

!SKIP s specifies how many lines are to be skipped before reading the regressor data,

!NONAMES indicates there is no line containing the individual names of the regressor variables; otherwise names are taken from the first (non-skipped) line in the file.

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If the factor identifiers are not present (!NOID), ASReml assumes that the order of the factor classes in the data file matches the order in the .grr file. If the factor identifiers are present, ASReml uses the identifiers obtained from the .grr file to define the order of the factor classes when the data is read; any extra identifiers in the data not in the .grr file are appended at the end of the factor level name list. If !NOID is set, identifiers in the .grr file are not needed and if present should be skipped using !CSKIP.

Values are typically TAB, COMMA or SPACE separated but may be packed (no separator) when all values are integers  $0/1/2$ . Missing values in the regression variables may be represented by \*, NA. Invalid data is also treated as missing. Missing values are replaced by the mean of the respective regressor. Alternative missing data methods that involve imputation from neighbouring markers have not been implemented.

Some general qualifiers are:

!SAVEGIV instructs ASReml to write the  $G$  matrix in .dgiv format,

!PSD s declares that the derived variance matrix may have up to s singularities,

!PEV requests calculation of Prediction Error Variance of marker effects which are reported in the .mef file. Calculation of prediction error variances was computationally very expensive. The algorithm has been drastically improved and now the recommendation is to always use !PEV.

! CENTRE  $[c]$  requests ASReml to centre the regressors at c if c is specified else at the individual regressor means; otherwise the  $G$  matrix is formed from uncentered regressors. Note that centring introduces a singularity in the G matrix and !PSV s will need to be set.

Other qualifiers relate specifically to whether the regressors are markers. Markers are typically coded  $0/1/2$  being counts of the minor allele. However, if they are imputed, they will take real values between 0 and 2. Since marker files may be huge,

**!SMODE** b sets the storage mode for the regressor data, indicating whether it is marker data:  $b = 2$  sets 2bit storage for strictly  $0/1/2$  marker data,  $b = 8$  (the default) sets 8bit storage useful for marker data with imputed values having 2 digits after the decimal,  $b = 16$  sets 16bit storage useful for marker data with imputation with more than 2 digits and  $b = 32$ sets 32bit real storage and should be used for non-marker data,

**!RANGE** l h indicates the marker scores range  $l : h$  and are to be transformed to have a range 0:2,

!GSCALE s, controls the scaling of the GRM matrix. If unspecified  $s = \sum 2p(1-p)$  is used for marker data,  $s = 1$  for non marker data (!SMODE 32). Scaling is often used with centred marker data to scale the  $MM'$  matrix so that it is a genomic relationship matrix.

#### Example

```
!WORK 1
Nassau Clone Data
 Nfam 71 !A
Nfemale 26 !A
 Nmale 37 !A
```

```
Clone !A 860
 rep 8 !A
 iblk 80 !A
 tree
 row
 col
 prop 1 !A
 culture 2 !A
 treat 2 !A
 measure 1 !A
 SURV
 DBH6
 HT6
 HT8
 CWAC6 !M-9
snpData.grr Clone !SKIP 1 !HEAD 0 !CENTRE !MARKERS 4854 !IDS 923 !PEV
nassau cut v3.csv !MAXIT 30 !SKIP 1 !GDENSE !PEV
HT6 ∼ mu culture culture.rep !r grm1(Clone) Clone rep.iblk
where snpData.grr is first used to declare Clone identifiers (taken from the first field) in
the correct order, and then contains the marker scores; it looks like
Genotype, 0-10024-01-114, 0-10037-01-257, 0-10040-02-394,...
```

```
140099,2,2,1,2,2,2,2,2,2,1,2,1,2,1,1,2,1,2,2,2,2,2,1,2...
141099,2,2,0,0,2,2,1,2,2,1,2,1,2,2,0,2,2,2,2,1,2,2,1,1...
...
547853,2,2,1,2,2,2,1,2,2,0,2,1,2,2,2,2,2,2,2,1,2,...
547966, 2, 2, 1, 1, 1, 2, 0, 2, 2, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 2, \ldots548082,2,2,1,2,2,2,1,2,1,2,2,1,2,2,1,2,2,2,2,1,2,...
```
The primary output follows:

```
Nfam 71 !A
Nfemale 26 !A
Nmale 37 !A
Clone !A 860
MatOrder 914 !A
rep 8 !A
iblk 80 !A
prop 1 !A
culture 2 !A
treat 2 !A
measure 1 !A
CWAC6 !M-9
Parsing: snpData.grr Clone !SKIP 1 !HEAD 0 !CENTRE !IDS 923 !PEV
```
Class names for factor "Clone" are initialized from the .grr file. Notice: SNP data line begins: 140099,2,2,1,2,2,2,2,2,2,1,2,1,2,1,1, Notice: Markers coded -9 treated as missing. Marker data  $[0/1/2]$  for 923 genotypes and 4854 markers read from snpData.grr 160414 missing Regressor values ( 3.6%) replaced by column average! Regressor values ranged 0.00 to 2.00 Regressor Means ranged 1.00 to 2.00 Regressors centered at their respective means Sigma2p(1-p) is 1057.12558 GIV1 snpData.grr 923 9 -963.89 QUALIFIERS: !MAXIT 30 !SKIP 1 !GDENSE QUALIFIER: !DOPART 3 is active Reading nassau\_cut\_v3.csv FREE FORMAT skipping 1 lines Univariate analysis of HT6 Summary of 6399 records retained of 6795 read Model term Size #miss #zero MinNon0 Mean MaxNon0 StndDevn 1 0 0 1 36.3379<br>26 0 0 1 12.8823 2 Nfemale 26 0 0 1 12.8823 26<br>3 Nmale 37 0 0 1 15.2285 37 37 0 0 1 15.2285 37 Warning: More levels found in Clone than specified 4 Clone 926 0 0 1 464.6765 926 Warning: Fewer levels found in MatOrder than specified 5 Mat0rder 914 0 0 1 432.5760 860 6 rep 8 0 0 1 4.4837 8 7 iblk 80 0 0 1 40.1164 80 8 tree  $0$  0 1.0000 7.473 14.00 4.018 9 row 0 0 1.0000 28.52 56.00 16.09 10 col 0 0 1.0000 10.50 20.00 5.760 Warning: Fewer levels found in prop than specified 11 prop 1 2 0 0 1 1.0000 1 12 culture 2 0 0 1 1.4945 2 13 treat 1.4945 2 2 0 0 1 1.4945 2 Warning: Fewer levels found in measure than specified 14 measure 2 0 0 1 1.0000 1 15 SURV 0 6 1.0000 0.9991 1.0000 0.3061E-01 16 DBH6 4 0 0.3000E-01 11.29 18.80 2.400 17 HT6 Variate 0 0 76.20 838.6 1286. 163.6 18 HT8 83 0 91.44 1148. 1576. 170.6 19 CWAC6 3167 0 97.54 301.3 542.5 52.26 20 mu 1 21 culture.rep 16 12 culture : 2 6 rep : 8 Warning: GRM matrix is too SMALL 22 grm1(Clone) 923 23 rep.iblk 640 6 rep : 8 7 iblk : 80 Notice: Random model term grm1(Clone) is included in the DENSE equations. Use !GDENSE -1 before model line to cancel this action. Notice: This job may require more workspace. Forming 2508 equations: 942 dense. Initial updates will be shrunk by factor 0.316 Notice: LogL values are reported relative to a base of -30000.000 Notice: 11 singularities detected in design matrix. 1 LogL=-2844.04 S2= 8959.5 6391 df 2 LogL=-2797.00 S2= 8569.9 6391 df



Notes:

- of 926 clones identified, 860 have data and 923 have genomic data.
- The .res file contains additional details about the analysis including a listing of the larger marker effects. All marker effects are reported in the .mef file.
- Particular columns of the .grr data can be included in the model using the  $grr(Factor, i)$ model term where and i specifies which (number) regressor variable to include.



### <span id="page-24-0"></span>1.2.7 Functions of variance components

Two new functions have been introduced to allow multiplication of parameters and taking square roots of parameters and calculating standard errors of these functions.

S *label i:j* when *i:j* are assumed positive variance parameters, inserts components which are the **SQRT** of components  $i:j$ ,

X label  $i^*k$  inserts a component being the product of components i and k.

X *label i:j\*k* inserts  $j - i + 1$  components being the products of components  $i : j$  and k.

X *label i:j\*k:l* inserts a set of  $j-i+1$  components being the pairwise products of components  $i : j$  and  $k : l$ .

The multiply option (X) allows a correlation in a CORUV structure to be converted to a covariance. The SQRT option allows conversion of CORGH to US, provided the dimension is moderate (say  $< 10$ ).

One can also convert CORUH and XFA to US using

V *label i:j* where  $i : j$  spans an XFA variance structure, inserts the US matrix based on the XFA parameters.

V label i:j where i: j spans a CORUH variance structure, inserts the US matrix based on the CORUH parameters.

When ASReml reads back the variance parameters from the .asr file, the parameters are given a name based on the random linear model term. The parameters in the R structures are effectively given a name Residual. The individual variance parameters associated with the linear model term can be specified by number, or sequence of numbers  $(n : m)$  by appending these in square braces after the linear model term, for example C.Trait[3] or Residual[ 4:6]. Users may contract names if they do not cause ambiguity, for example Sire.Trait might be contracted to Sire if there are no other random terms including Sire. If the user is in doubt of the name or number of a parameter then running the program with VPREDICT !DEFINE and a blank line will construct a .pvc file with the names and numbers of parameters identified.

**Critical change** For generalised linear models in ASReml 4 the . pvc file reports and numbers, for completeness, a residual or dispersion parameter both when the parameter is estimated or fixed. By contrast ASReml 3 does not report or number if the parameter is fixed, by default, at 1. Hence the parameters might be numbered differently in ASReml 4 and ASReml 3.

#### <span id="page-25-0"></span>1.2.8 A detailed example

...

The following example for a **bivariate sire model** is a little more complicated. The job file bsiremod.as contains

```
coop.fmt
ywt fat ~ Trait Trait.(age c(brr) sex sex.age) !r Trait.sire !f Tr.grp
1 2 1
0 0 ID
Trait 0 US * !GP
Trait.sire 2
Trait 0 US * !GP
sire 0 ID
VPREDICT !DEFINE
F phenvar Residual + Sire; Trait \begin{array}{ccc} \hbox{#} & 1:3 + 4:6 \\ \hbox{F} & \hbox{addvar} & \hbox{sire} \end{array} + 4
F addvar sire * 4 \text{# } 4:6 * 4:6 * 4 \text{# } 4:6 * 4:6 * 4 \text{# } 4:7H heritA addvar[1] phenvar[1]
H heritB addvar[3] phenvar[3] \qquad # 12 9<br>R phencorr phenvar \qquad # 7 8 9
R phencorr phenvar \begin{array}{ccc} \hline \text{R} & \text{p} \\ \text{R} & \text{q} \\ \text{R} & \text{q} \\ \hline \end{array} # 7 8
R gencorr addvar
```
The relevant lines of the .asr file are



Numbering the parameters reported in bsiremod.asr (and bsiremod.vvp)

```
error variance for ywt
error covariance for ywt and fat
error variance for fat
sire variance component for ywt
```
- 5 sire covariance for ywt and fat
- 6 sire variance for fat

then

```
F phenvar Residual + Trait.sire or
F phenvar Residual + sire; Trait or F phenvar 1:3 + 4:6
```
creates new components  $7 = 1+4$ ,  $8 = 2+5$  and  $9 = 3+6$ ,

F addvar sire; Trait  $*$  4 or F addvar 4:6  $*$  4

creates new components  $10 = 4 \times 4$ ,  $11 = 5 \times 4$  and  $12 = 6 \times 4$ ,

H heritA addvar[1] phenvar[1] **bleef** and the set of H heritA 10 7

forms  $10 / 7$  to give the heritability for ywt,



The resulting .pvc file contains:



<span id="page-26-0"></span>The first 8 lines are based on the .asr file.

#### 1.2.9 Updating loadings in factor analytic models

The algorithm for updating loadings in factor analytic models has been improved. This builds on an earlier change implemented in ASReml 4 which modified updates to loadings, but proved too conservative causing such jobs to take too many iterations to converge. The motivation for change was that the original update procedure sometimes produced unreasonable updates, or otherwise came near to convergence and then drifted away. The present procedure is to modify the average information matrix by increasing the diagonal elements pertaining to loadings by a percentage, p. The default is to start with  $p = 10\%$  and reduce it by 1 or 2% each iteration down to 1%. If the starting values are poor, 10% may not be a sufficient initial retardation. If it appears the updates are unreasonable, ASReml will increase the value of p by  $10\%$  and then continue. The user can set the initial value of p with the qualifier !AIPENALTY p. After the penalty has reduced to  $1\%$ , it is further reduced to 0.2%. The qualifier can be used to set p to 0 if desired. The value of p can be monitored by using the !LOGFILE and !DEBUG command line qualifiers and searching the .asl file for the string XFAIF (XFA Inflation Factor).

## <span id="page-27-0"></span>1.3 Modifications and improvements to output

#### <span id="page-27-1"></span>1.3.1 Output formats in the .asr file

The general aim has been to make as few changes as possible to output formats. However, there are some minor changes with this release. These are likely to effect users who have developed in-house routines to parse ASReml output files. Some field widths have been changed to reduce the frequency of fields running together. In particular, the header line for the table of variance components has been changed to



and the contents of the leading fields modified to better identify the particular components. These now show the model term, the component (of an interaction) and the variance structure, the parameter type and the indexing or size information in a more consistent manner than before.

### <span id="page-27-2"></span>1.3.2 Writing out a design matrix

The new qualifier !DESIGN on the datafile line causes ASReml to write the design matrix, not including the response variable, to a .des file. It allows ASReml to create the design matrix required by the VCM process, see Section [1.2.1.](#page-14-3) For example, using a control file vcmdes.as containing

```
Create VCM Design for H-F model
Row *
Col *
\bigcap_{i=1}^{n}Y !=VO
vcmdes.asd !DESIGN
Y \sim \text{Row and}(\text{Row},-0.5) and(Col,0.5) Off
```
and a data file vcmdes.asd containing

1 1 0  $2 \t1 -1$ 

then the file vcmdes.des will be generated which contains the values used in fitting the variance model for the HuynhFeldt model given in Section [1.2.1.](#page-14-3)

## <span id="page-28-0"></span>1.3.3 XML output

The primary tables reported in the .asr file and key output from .pvs and .sln files are written to .xml file in xml format. Output is presented in the order of computation. The first block written is a .asr block includes start and finish times, the data summary, the iteration sequence summary and information criteria, then from the .pvs file the tables and associated information, then the summary of estimated variance structure parameters from the .asr file, then information from the .sln file then finally the Wald F statistics and completion information from the .asr file. The process is repeated for each cycle of analysis. The intended use of this file is by programs written to parse ASReml output. For further details, including the status of intended future developments, please contact support@vsni.co.uk.

## <span id="page-28-1"></span>1.3.4 Writing output to a separate folder

!OUTFOLDER [path] allows most of the output files to be written to a folder other than the working folder. This qualifier must be placed on the top command line as it needs to be processed before any output files are opened. Most files produced by ASReml have a filename structure

 $<$ basename $>$  $<$ subname $>$ . $<$ extension $>$ 

where  $\langle$ *subname* $\rangle$  is a command line argument value. If **!OUTFOLDER** is specified without path, the output filename pattern becomes

 $<$ basename> $<$ subname> $/$  $<$ basename>. $<$ extension>

If path is specified, the output filename pattern becomes

 $\langle path \rangle / \langle basename \rangle \langle subname \rangle. \langle extension \rangle$ 

There are a few files written by ASReml that do not follow this naming pattern, for example, ainverse.bin and asrdata.bin. These remain unchanged, that is, they are not written to the output folder.

## <span id="page-29-0"></span>1.3.5 Prediction using two-way interaction effects

In some cases we wish to calculate from two way interaction effects,  $bc_{ij}$  say, effects for one of the factors,  $\bf{B}$  say, that are a weighted sum averaged over the c levels of  $\bf{C}$ , ie.  $b_i = \sum_{j=1}^c b c_{ij} w_j.$ 

TPREDICT C !AVE B weights !ONLYUSE B.C

allows this to be produced more computationally efficiently than it would be using PREDICT. For example,

TPREDICT Animal !AVE Trait 2.1 1.2 -7.4 !ONLYUSE Trait.Animal

Part of the motivation for this is the calculation of selection indices. The index coefficients are typically derived as  $w = a' G_{om} G_{mm}^{-1}$  where  $G_{mm}$  is the variance matrix for the measured traits (corresponding to  $C$  in the example),  $G_{om}$  is the genetic covariance matrix between the objective traits and the measured traits, and  $a$  is the vector of economic values for the objective traits. The results are given in a .sli (selection index) file. This directive should be placed after the model specification.

## <span id="page-29-1"></span>1.3.6 Solution (.sln) file

A header

```
Model_Term Level Effect seEffect
```
has been added. Note that extra significant digits are reported when **SLNFORM** is set, and expanded labelling of the levels in interactions is used because field width is no longer restricted.

# <span id="page-29-2"></span>1.4 Functional specification of the mixed model

The main development in Release 4 is the implementation of a functional model specification. This is described in detail in Chapter [2.](#page-30-0) The distinguishing feature of this specification is that the variance models for individual terms are specified by applying variance model functions to the terms in the model definition lines. This is in contrast to the structural specification of versions prior to Release 4 in which the variance models were only imposed after the mixed model definition line(s).

The functional specification is described through a series of examples of increasing complexity, using the Nebraska Intrastate Nursery (NIN) data (Chapter 3 of the User Guide) for demonstration. A more comprehensive set of examples is presented in Chapter [3.](#page-69-0)

# <span id="page-30-0"></span>2 Functional specification of the mixed model

## <span id="page-30-1"></span>2.1 Introduction

Prior to Release 4, variance structures were applied to random model terms and the residual error term by specifying these structures after the mixed model had been specified. In Release 4, a new functional specification of the variance model has been implemented in which variance structures can be specified by applying variance model functions directly to terms in the model definition line(s). This offers a more concise and less error-prone alternative to the structural specification and mirrors the implementation in ASReml-R. An understanding of the new specification should facilitate free movement between the standalone and R platforms.

The functional specification is introduced for the random model terms in Section [2.4](#page-34-1) and the residual error term in Section [2.5.](#page-39-0) In Section [2.7](#page-44-0) the NIN data is used for demonstration, with coding included for both specifications to allow direct comparison between the existing and new code. More advanced aspects of the functional specification are presented after the example.

## <span id="page-30-2"></span>2.2 Typographic convention

A box system is used to assist existing users in migrating from the structural specification to the functional specification that is new with Release 4:

Boxes like this are used throughout this chapter to present the structural specification corresponding to the particular aspect of the functional specification under discussion.

## <span id="page-30-3"></span>2.3 The theory

From Chapter 2 of the ASReml User Guide, the linear mixed model can be written as

<span id="page-30-4"></span>
$$
y = X\tau + Zu + e \tag{2.1}
$$

where y  $(n \times 1)$  is a vector of observations,  $\tau$   $(p \times 1)$  is a vector of fixed effects,  $\boldsymbol{X}$   $(n \times p)$ is the design matrix of full column rank that associates observations with the appropriate combination of fixed effects,  $u$  ( $q \times 1$ ) is a vector of random effects,  $\mathbf{Z}$  ( $n \times q$ ) is the design matrix that associates observations with the appropriate combination of random effects, and  $e(n \times 1)$  is the vector of residual errors.

#### <span id="page-31-0"></span>2.3.1 Sigma parameterization of the linear mixed model

Model [\(2.1\)](#page-30-4) is called a linear mixed model or linear mixed effects model. It is assumed

<span id="page-31-4"></span>
$$
\begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{e} \end{bmatrix} \sim N \left( \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{0} \end{bmatrix}, \begin{bmatrix} \boldsymbol{G}(\boldsymbol{\sigma}_g) & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{R}_v(\boldsymbol{\sigma}_r) \end{bmatrix} \right) \tag{2.2}
$$

where the matrices G and  $R_v$  are variance matrices for u and e and are functions of parameters  $\sigma_q$  and  $\sigma_r$ . This requires that the random effects u and residual errors e are uncorrelated. The variance matrix for  $y$  is then of the form

<span id="page-31-2"></span>
$$
var(\boldsymbol{y}) = \boldsymbol{Z}\boldsymbol{G}(\boldsymbol{\sigma}_g)\boldsymbol{Z}^{\mathsf{T}} + \boldsymbol{R}_v(\boldsymbol{\sigma}_r) \qquad (2.3)
$$

which we will refer to as the *sigma parameterization* of the G and R variance structures, and the individual variance structure parameters in  $\sigma_q$  and  $\sigma_r$  will be referred to as *sigmas*. The variance models given by  $G$  and  $R_v$  are referred to as G structures and R structures respectively.

We illustrate these concepts using the simplest linear mixed model, that is, the one-way classification.

#### <span id="page-31-3"></span>Example 2.1 A simple example

Consider a one-way classification comprising a single random effect  $u$ , and a residual error term  $e$ . The two random components of this model, namely  $u$  and  $e$ , are assumed to be independent and to follow a normal distribution such that  $u \sim N(0, \sigma_u^2 I_q)$  and  $e \sim$  $N(\mathbf{0}, \sigma_e^2 \mathbf{I}_n)$ . Hence the variance of **y** has the form

$$
var(\boldsymbol{y}) = \sigma_u^2 \boldsymbol{Z} \boldsymbol{Z}^{\mathsf{T}} + \sigma_e^2 \boldsymbol{I}_n \tag{2.4}
$$

This model has two variance structure parameters or sigmas: the variance component  $\sigma_u^2$ associated with  $u$ , and the variance component  $\sigma_e^2$  associated with  $e$ . Mapping this equation back to [\(2.3\)](#page-31-2), we have  $\boldsymbol{\sigma}_g = \sigma_u^2$ ,  $\boldsymbol{G}(\boldsymbol{\sigma}_g) = \sigma_u^2 \boldsymbol{I}_q$ ,  $\boldsymbol{\sigma}_r = \sigma_e^2$  and  $\boldsymbol{R}_v(\boldsymbol{\sigma}_r) = \sigma_e^2 \boldsymbol{I}_n$ .

<span id="page-31-1"></span> $\Box$ 

#### 2.3.2 Partitioning the fixed and random model terms

Typically,  $\tau$  and **u** are composed of several model terms, that is,  $\tau$  can be partitioned as  $\boldsymbol{\tau}^{\top} = \begin{bmatrix} \boldsymbol{\tau}^{\intercal}_1 \end{bmatrix}$  $\mathsf{T} \mathsf{T}_1 \ldots \boldsymbol{\tau}_t^\intercal$  $\mathbf{u}_{t}^{\text{[t]}}$  and **u** can be partitioned as  $\mathbf{u} = [\mathbf{u}_{t}^{\text{[t]}}]$  $\frac{\mathbf{I}}{\mathbf{I}} \ldots \overset{\mathbf{I}}{\bm{u}}^{\mathsf{T}}_{b}$  $\mathbf{X}_{b}$ <sup>T</sup>, with **X** and **Z** partitioned conformably as  $\boldsymbol{X} = [\boldsymbol{X}_1 \dots \boldsymbol{X}_t]$  and  $\boldsymbol{Z} = [\boldsymbol{Z}_1 \dots \boldsymbol{Z}_b]$ .

#### <span id="page-32-0"></span>2.3.3 G structure for the random model terms

For **u** partitioned as  $u = [u]$  $\frac{1}{1} \ldots \bm{u}_b^{\intercal}$  $\mathbf{G}_{b}^{\text{t}}$ , we impose a direct sum structure on the matrix  $\boldsymbol{G}_{b}$ , written

$$
\mathbf{G} = \bigoplus_{i=1}^{b'} \mathbf{G}_i = \left[ \begin{array}{cccc} \mathbf{G}_1 & 0 & \dots & 0 & 0 \\ 0 & \mathbf{G}_2 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \mathbf{G}_{b'-1} & 0 \\ 0 & 0 & \dots & 0 & \mathbf{G}_{b'} \end{array} \right]
$$

where  $\oplus$  is the direct sum operator, each  $G_i$  is of size  $q_i$  and  $q = \sum_i q_i$ .

The default assumption is that each random model term generates one component of this direct sum (then  $b' = b$  and var  $(u_i) = G_i$  for  $i = 1...b$ ). This means that the random effects from any two distinct model terms are uncorrelated. However, in some models, one component of  $\boldsymbol{G}$  may apply across several model terms, for example, in random coefficient regression where the random intercepts and slopes for subjects are correlated, see [2.4.2.](#page-36-0) To accommodate these cases, one component of  $G$  may apply across several model terms (then  $b' < b$ ). In some other (less likely but possible) cases, we may wish to separate one model term over several independent parts (then  $b' > b$ ), see Section [2.4.2.](#page-36-0)

#### Example 2.2 Variance components mixed models

Building example [2.1](#page-31-3) to a linear mixed model with more than one  $(b > 1)$  random effect (typically known as a variance components mixed model), the random effects  $u_i$  in  $u_j$ , and the residual errors e, are assumed pairwise uncorrelated and to each be normally distributed with mean zero and variance given by

$$
\text{var}\left(\bm{u}_{i}\right) \hspace{0.1cm} = \hspace{0.1cm} \sigma_{u_{i}}^{2} \bm{I}_{q_{i}}
$$

and

$$
\text{var}(\boldsymbol{e}) = \sigma_e^2 \boldsymbol{I}_n
$$

where  $I_{q_i}$  and  $I_n$  are identity matrices of dimension  $q_i$  and n, respectively. In this case

<span id="page-32-2"></span>
$$
\operatorname{var}(\boldsymbol{y}) = \sum_{i=1}^{b} \sigma_{u_i}^2 \boldsymbol{Z}_i \boldsymbol{Z}_i^{\mathsf{T}} + \sigma_e^2 \boldsymbol{I}_n. \tag{2.5}
$$

<span id="page-32-1"></span> $\Box$ 

#### 2.3.4 Partitioning the residual error term

As for the fixed and random model terms, it is often useful or appropriate to consider a partitioning of the vector of residual errors e according to some conditioning factor. We use the term section to describe this partitioning and the most common example of the use of sections in  $e$  is when we wish to allow sections in the data to have different variance structures. For example, in the analysis of multi-environment trials (METs) it is natural to expect that each trial will require a separate (possibly spatial) error structure. In this case, for s sections we have  $e = [e_1^{\mathsf{T}}]$  $_{1}^{\intercal},\bm{e}_{2}^{\intercal}$  $\frac{1}{2},\ldots,\bm{e}_s^{\intercal}$  $\int_{s}^{T}$ ]<sup>T</sup> assuming that the data vector is ordered by section, and where  $e_j$  represents the vector of errors for the  $j<sup>th</sup>$  section.

#### <span id="page-33-0"></span>2.3.5 R structure for the residual error term

For **e** partitioned as  $e = [e_1]$  $_{1}^{\intercal},\boldsymbol{e}_{2}^{\intercal}$  $\frac{1}{2},\ldots,\bm{e}_s^{\intercal}$  $_s^{\text{II}}$  we allow the matrix  $\boldsymbol{R}_v$  to have a similar direct sum structure, with



for  $s \geq 1$  sections and the data ordered by section. Note that it may be necessary to reorder (re-number) the data units in order to achieve this structure. In ASReml it is now straightforward to apply possibly different variance structures to each component of  $\mathbf{R}_v$ .

In many cases, the residual errors  $(e)$  can be expected to share a common variance structure. In this case there is only one section  $(s = 1)$ .

Typically a variance structure is specified for each random model term and often more complex models than the simple IID model are specified. ASReml offers a wide range of variance models to choose from. They are listed in Table [2.5](#page-61-1) and are described in more detail in the following sections.

#### <span id="page-33-1"></span>2.3.6 Gamma parameterization for the linear mixed model

The sigma parameterization of model  $(2.3)$  is one possible parameterization of var  $(y)$ . In this parameterization both  $G(\sigma_q)$  and  $R_v(\sigma_r)$  are variance matrices and the variance structure parameters in  $\sigma_q$  and  $\sigma_r$  are referred to as *sigmas*, see above. Other parameterizations are possible and are sometimes useful. For example, in some of the early development of REML for the traditional mixed model of [\(2.5\)](#page-32-2), the variance matrix was parameterized as the equivalent model

$$
\text{var}(\boldsymbol{y}) = \sigma_e^2 \left( \sum_i^b \gamma_{g_i} \boldsymbol{Z}_i \boldsymbol{Z}_i^{\mathsf{T}} + \boldsymbol{I}_n \right) \tag{2.6}
$$

for  $\gamma_{g_i}$  being the ratio of the variance component for the random term  $u_i$  relative to error variance, that is,  $\gamma_{g_i} = \sigma_{u_i}^2/\sigma_e^2$ . In this case ASReml calculated a simple estimate of  $\sigma_e^2$  and initial values for the iterative process were specified in terms of the ratios  $\gamma_{g_i}$  rather than in

terms of the variance components  $\sigma_{u_i}^2$ . It was often easier to specify initial values in terms of these ratios rather than the variance components which is why this approach was adopted. Where  $\mathbf{R}_v(\sigma_r)$  can be written as a scaled correlation matrix, that is,  $\mathbf{R}_v(\sigma_r) = \sigma_e^2 \mathbf{R}_c(\gamma_r)$ , this suggests the alternative specification of  $(2.2)$ 

$$
\begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{e} \end{bmatrix} \sim N \left( \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{0} \end{bmatrix}, \ \sigma_e^2 \begin{bmatrix} \boldsymbol{G}(\boldsymbol{\gamma}_g) & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{R}_c(\boldsymbol{\gamma}_r) \end{bmatrix} \right) \tag{2.7}
$$

where  $\gamma_g$  and  $\gamma_r$  represent the variance structure parameters associated with scaled (by  $\sigma_e^2$ ) variance matrices. In this case

<span id="page-34-2"></span>
$$
\text{var}(\boldsymbol{y}) = \sigma_e^2 \left( \boldsymbol{Z} \boldsymbol{G}(\boldsymbol{\gamma}_g) \boldsymbol{Z}^\mathsf{T} + \boldsymbol{R}_c(\boldsymbol{\gamma}_r) \right), \tag{2.8}
$$

which we will refer to as the *gamma parameterization*, and the individual variance structure parameters in  $\gamma_q$  and  $\gamma_r$  will be referred to as *gammas*. ASReml switches between the sigma and gamma parameterizations for estimation. This is discussed further in Section [2.8.](#page-52-0)

#### <span id="page-34-0"></span>2.3.7 Parameter types

Each sigma in  $\sigma_q$  and  $\sigma_r$  and each gamma in  $\gamma_q$  and  $\gamma_r$  has a parameter type, for example, variance components, variance component ratios, autocorrelation parameters, factor loadings. Furthermore, the parameters in  $\sigma_g$ ,  $\sigma_r$ ,  $\gamma_g$  and  $\gamma_r$  can span multiple types. For example, the spatial analysis of a simple column trial would involve variance components (sigma parameterization) or variance component ratios (gamma parameterization) and spatial autocorrelation parameters.

Parameterization prior to Release 4 When ASReml was developed, [\(2.2\)](#page-31-4) and [\(2.8\)](#page-34-2) were combined into  $\lceil u$ e  $\Big] \sim N \Big( \Big[ \, \begin{matrix} 0 \\ 0 \end{matrix} \Big]$ 0  $\Big] \, , \; \theta \, \Big[ \begin{array}{cc} G(\gamma) & 0 \ 0 & D(\gamma) \end{array} \Big]$  $\begin{pmatrix} \n\sqrt{2} & \mathbf{0} \\
\mathbf{0} & \mathbf{R}(\boldsymbol{\phi})\n\end{pmatrix}$ (2.9)

where  $\theta$  was referred to as a scaling parameter and was used in specifying the variance model. The way  $\theta$  was treated depended on the way  $R(\phi)$  was defined. If  $R(\phi)$  included variance parameters then, to avoid problems in estimability and for convenience, we set  $\theta = 1$ . In this case, ASReml used the sigma parameterization and estimated sigmas were reported. Alternatively, if  $\mathbf{R}(\phi)$  was defined to be a correlation matrix (diagonal elements equal to 1) then the gamma parameterization was used and the estimated gammas were reported. In this case the estimated sigmas were also reported.

## <span id="page-34-1"></span>2.4 Applying variance structures to random model terms

The random model terms  $u_i$  in  $u$  define the random effects and associated design matrices,  $\mathbf{Z}_i \in \mathbf{Z}$ , but additional information is required before the model can be fitted. This extra step involves defining the G structure for each term. In general, there are two different approaches to this problem which we refer to as the structural approach and the functional approach. The structural approach applies variance models to individual terms after the

random model has been defined. This has been the approach of ASReml until Release 4 and gives a step-by-step approach to building up the full model that is straightforward but not concise. In contrast, the functional approach that is new to Release 4, uses functions to directly apply variance models to the components of the random model term to produce a consolidated model term that simultaneously defines both the design matrix  $(Z_i)$  and variance model  $(G_i)$ .

#### <span id="page-35-0"></span>2.4.1 Process to define a consolidated model term

Consider a linear model term column.row comprising the interaction between the single model terms column and row. We refer to column.row as a *compound model term*. If the variance structure for column.row is the direct product of two matrices, the first of which is an IID variance structure that is a scaled identity matrix with dimension equal to the number of levels of the factor column and the second of which is a matrix with dimension equal to the number of levels of the factor row and with elements representing a first order autoregressive correlation structure AR1, then we represent this by the consolidated model term idv(column).ar1(row). This specifies a two-dimensional separable spatial variance structure for column.row but with spatial correlation in the row direction only. A consolidated model term is therefore comprised of component terms, each with a variance model function applied to give the required direct product form of the variance structure. Table [2.1](#page-36-1) demonstrates how to build consolidated terms in ASReml for a small selection of examples. The linear model term (single or compound) is first identified (*column 2*) and the individual components that identify the dimension of the individual matrices used in forming the direct product variance structure are then written down (column 3). Note that in the simplest cases there is only one component. The variance structure associated with each component has a structure name (column 4) and a corresponding variance model function name (column 5) giving the associated component variance structures (*column 6*). The consolidated model term is the term presented in the final column of the table. In contrast, in ASReml 3 the linear model terms are defined on the model line and subsequently a G structure line is given for each linear model term which specifies the component terms and their associated structures. The simplest form of a consolidated model term is a single model term with a variance model function applied, eg. idv(repl) in Table [2.1,](#page-36-1) and the next simplest is a compound model term with a variance model function applied, eg.  $\texttt{idv}(A.B)$  in Table [2.1.](#page-36-1)

In summary, the following are rules in forming consolidated model terms and applying variance model functions to random model terms:

- variance model functions can be applied to single model terms (see example 1 in Table [2.1\)](#page-36-1), the components in compound model terms (examples 4 to 6) and constructed linear model functions of variables (example 2),
- variance model functions can also be applied to compound model terms (example 3)
- variance model functions *cannot* be applied to expandable model terms, for example, to  $- A*B$  which expands to  $A$  B  $A$ . B
- $A/B$  which expands to  $A$   $A$ . B
- $at(A,i,j)$ .B which expands to  $at(A,i)$ .B  $at(A,j)$ .B
- only one component of a variance structure for a compound model term may include a variance parameter, the other components must be correlation structures (no associated variance parameter). This is due to the identifiability issues that occur when multiple variance structures are specified. This is explained in NIN example 3a, see Section [2.7.](#page-44-0) The defined variance function may be homogeneous (name ending in v) or heterogeneous variance (name ending in h). This is discussed in detail in Section 2.4 of the User Guide.

<span id="page-36-0"></span>Some common variance functions are defined in Table [2.2;](#page-37-0) the full range of variance model functions and their detailed definition is presented in Table [2.5.](#page-61-0)



#### Table 2.1: Building consolidated model terms in ASReml

### 2.4.2 Modelling a single variance structure over several model terms

This facility was motivated by two considerations. Typically the random effects from any two distinct model terms are uncorrelated. However, in some models one G structure may apply across several model terms. Sometimes one also wishes to partition the random effects into sets with independent variance structures. In ASReml, we can accomplish these two models using the special variance model function  $str()$ , where the name  $str$  is for *structure* and str() has the following general form:

<span id="page-37-0"></span>Table 2.2: List of common variance model functions, their type (correlation or variance), the form of the variance matrix generated  $(C$  for correlation,  $V$  for variance matrix), and a brief description. Parameters  $\sigma_i^2 > 0$  are variances,  $-1 < \rho_i < 1$  are correlations. Subscipt c denotes parameter held in common across all rows/columns.

name	type	variance matrix (for set of $n$ effects)	description
id()	correlation	$C = I$	<b>ID</b> with variance 1
idv()	variance	$\boldsymbol{V} = \sigma_c^2 \boldsymbol{I}$	$\text{IID}$ with common variance $=$ default model
idh()	variance	$V = \text{diag}\lbrace \sigma_1^2 \dots \sigma_n^2 \rbrace$	independent with separate variances
ar1()	correlation	$C_{ij} = \rho_c^{ i-j }$	auto-regressive structure of order 1
ar1v()	variance	$V_{ij} = \sigma_c^2 \rho_c^{ i-j }$	auto-regressive structure of order 1
ar1h()	variance	$V_{ij} = \sigma_i \sigma_j \rho_c^{ i-j }$	auto-regressive structure of order 1
$\text{corg}()$	correlation	$C_{ij} = \rho_{ij}$	unstructured correlation matrix
diag()	variance	$V = \text{diag}\{\sigma_1^2 \dots \sigma_n^2\}$	independent with separate variances (same as $idh()$ )
grm()	$(known)$ cor- relation	$C$ specified	applies a known (scaled) correlation matrix; the number of rows in the matrix must be match the number of levels of the factor it is applied to and the order of rows must match the order of the levels
nrm()	$(known)$ cor- relation	$C$ specified	applies a generated relationship matrix derived from the functions argument associated pedigree file
us()	variance	$V_{ij} = \sigma_{ij}$	general unstructured, symmetric positive definite co- variance matrix
fa(,k)	variance	$\boldsymbol{V} = \boldsymbol{\Lambda}\boldsymbol{\Lambda}^{\intercal} + \boldsymbol{\Psi}$	factor analytic model of order k with $\Lambda$ of size $n \times k$ .

#### $str(model term(s)$  variance structure(s))

The m individual model terms generate the design matrices  $\mathbf{Z}_i$  and effect vectors  $\mathbf{u}_i$  of size  $b_i$  (i=1,...,m) and the v variance structure terms generate variance structures  $\mathbf{G}_i$  of size  $b_j^*$   $(j = 1, ..., v)$ . The function str() generates a combined model design matrix  $\boldsymbol{Z}_c = [\boldsymbol{Z}_1 \dots \boldsymbol{Z}_m]$  and a combined effects vector  $\boldsymbol{u}_c^{\text{T}} = [\boldsymbol{u}_1^{\text{T}}]$  $\mathbf{u}_{1}^{\mathsf{T}} \dots \mathbf{u}_{m}^{\mathsf{T}}$  of size  $b_{c} = \sum_{i=1}^{m} b_{i}$  and the variance structure for  $u_c$  is  $G_c = \bigoplus_{j=1}^v G_j$  for  $u_c$  and  $G_c$  to be conformable  $\Sigma_{j=1}^v b_j^* = b_c$ . If  $v = 1$  then there is one variance structure associated with the combined set of effects and if  $v > 1$  we can partition  $u_c$  and  $G_c$  with  $u_c^{\dagger} = [u_1^*]$  $\mathbf{u}_i^*$ ,  $\mathbf{u}_v^*$ , and  $\mathbf{G}_c = [\mathbf{G}_1^*, \dots \mathbf{G}_v^*]$  and the effect vectors are independent of each other and the effects  $u_j^*$  have variance structure  $G_j^*$ . A restriction with str() is that the closing parenthesis must be on the same line because of the way ASReml processes the command file.

#### Example 2.3 Random coefficient regression

In the first order random coefficient regression model it is required to specify a covariance between the intercept and slope for each subject to ensure translation invariance, that is,

#### 2.4 Applying variance structures to random model terms

equivalent variance parameter estimates for addition of any constant to the independent variable. For example, in a random coefficient regression where a set of random intercepts is specified by the model term Animal (with 10 levels) and a set of random slopes is specified by the model term  $\text{age}$ . Animal, translation invariance is achieved using  $\text{str}()$  as

#### str(Animal age.Animal us(2).id(10))

The algorithm places the model terms specified using the argument form together in the processed random model, here Animal followed by age.Animal. The variance structure(s) begins at the start of the first term specified in str() and is expected to exactly span the whole set of terms given within the brackets. The overall size of the variance model is checked against the total number of levels of these terms, but the user must verify that the ordering is appropriate for (matches) the variance model specified.

Using the structural specification, the model term is written as !{ Animal age.Animal !} ... and the G structure lines as Animal 2 2 0 US 0.3 0.01 0.2 Animal 0 ID The idea was to define a variance structure that is associated with effects in the linear model starting at the first term specified and exactly spanning the whole set of terms given inside the  $\{\}$   $\}$  brackets.

In our example, this random model generates a combined set of random effects from the individual animal intercepts,  $\boldsymbol{u}_I = (u_{I1} \dots u_{I10})^\mathsf{T}$  and animal slopes,  $\boldsymbol{u}_S = (u_{S1} \dots u_{S10})^\mathsf{T}$ , as  $\boldsymbol{u}_{IS}=(\boldsymbol{u}_{I}^{\intercal}\,\boldsymbol{u}_{S}^{\intercal}$  $\mathbf{F}_S$ <sup>T</sup>. The consolidated term then has variance structure of the form

$$
\text{var}(\boldsymbol{u}_{IS}) = \text{var}\left(\left[\begin{array}{c} \boldsymbol{u}_{I} \\ \boldsymbol{u}_{S} \end{array}\right]\right) = \left[\begin{array}{cc} \sigma_{II} & \sigma_{IS} \\ \sigma_{IS} & \sigma_{SS} \end{array}\right] \otimes \boldsymbol{I}_{10} = \left[\begin{array}{cc} \sigma_{II}\boldsymbol{I}_{10} & \sigma_{IS}\boldsymbol{I}_{10} \\ \sigma_{IS}\boldsymbol{I}_{10} & \sigma_{SS}\boldsymbol{I}_{10} \end{array}\right]
$$

Here, the set of animal intercepts has a common variance  $(\sigma_{II})$ , and the set of animal slopes has a (different) common variance  $(\sigma_{SS})$ . Intercepts and/or slopes from two different animals are independent, but the intercept and slope from any given animal have covariance  $\sigma_{IS}$  (or correlation  $\sigma_{IS}/\sqrt{\sigma_{II}\sigma_{SS}}$ ). In this context, we use integers as arguments to emphasize that the arguments are specifying the size of the variance structure. For this example, id(10) can be replaced by  $id(Animal)$ . In order to simplify processing of the  $str()$  arguments, ASReml expects at least 1 single term in the consolidated model term to be a variance model function with a dimension rather than a variable name as the argument, eg. us(2) in the example. Mostly this is quite natural as a suitable factor is not normally available to indicate the number of linear model terms being combined (2 in this example). The dummy integer function id(1) could be introduced to allow processing if the consolidated model term could be expressed using variable arguments, for example,

str(Mpar and(Fpar) id(1).idv(Mpar))

overlays the Mpar and Fpar design matrices and allows the resulting effects to be modelled with a single variance parameter.

 $\Box$ 

Example 2.4 Fitting a genetic covariance between direct and maternal effects

This example fits direct effects for two traits, but maternal effects for the first trait only

str(Trait.animal at(Trait,1).dam us(3).nrm(animal))

where animal and dam are coded using the pedigree file.

```
Using the structural specification, the model term is written as
\ldots ! { Trait.animal at (Trait, 1).dam ! } \ldotsand the G structure lines as
Trait.animal 2
3 0 US
0.3
0.01 0.2
0.01 0.01 0.2
animal 0 NRM #was AINV in ASReml 3
```
 $\Box$ 

A rather artificial example of using v greater than 1 is when we have 20 levels in a factor  $\bf{A}$ and wish to use one variance for the first 8 levels and another for the last 12 levels. Then

 $str(A idv(8) idv(12))$ 

<span id="page-39-0"></span>will do this.

## 2.5 Applying variance structures to the residual error term

In Release 4 the residual error term is also defined using a consolidated model term, and it now appears after a residual statement that has been introduced to specify the associated variance structure. We give five examples. Firstly, for the default situation of IID residual errors (1. in box on page  $34$ ), the error model definition line would be

residual idv(units)

This second example would specify a separable autoregressive spatial model of order 1  $(AR1\times AR1)$  for the observations from a trial arranged in a rectangular array indexed by the data variables column and row  $(2. \text{in box on page 34}).$  $(2. \text{in box on page 34}).$  $(2. \text{in box on page 34}).$  To apply this variance structure the observations would need to cover the whole grid, but it would not be necessary to pre-order the data file as rows within columns as ASReml uses the information in column and row to

#### 2.5 Applying variance structures to the residual error term

put the observations into the appropriate row within column order:

residual ar1v(column).ar1(row)

If there were 3 columns and 23 rows in the previous example, then this third example

residual ar1v(3).ar1(23)

would be an equivalent coding for the  $AR1\times AR1$  model using the dimensions of the factors rather than the factor names (3. in box on page  $3/4$ ). In this case the data records would need to be sorted in the order rows within columns because ASReml does not have the information needed to reorder the data internally.

The fourth example assumes variance heterogeneity among the data observations, that is, that the three groups comprising observations  $1 \dots 23$ ,  $24 \dots 50$ ,  $51 \dots 70$  have unequal variances  $(4. \text{in box on page } 34)$  $(4. \text{in box on page } 34)$  $(4. \text{in box on page } 34)$ :

residual  $idv(23)$   $idv(27)$   $idv(20)$ 

The fifth and final example is the default residual variance in a multivariate analysis  $(5. \text{in})$ box on page  $34$ ). Specifying units as the first component is crucial as ASReml extracts the trait values by trait within unit:

residual id(units).us(Trait)

#### 2.5 Applying variance structures to the residual error term

In the structural specification the R structure is specified by a Variance header line consisting of three numbers  $s \, c \, g$ , followed by  $s$  sets of  $c$  variance structure lines.  $s$  is the number of sections (see below), c is the number of components in the R structure for each section, and  $q$ is the number of model terms with G structure definitions (described in the preceding section).

The following examples match the examples above as per the common italicized model descriptions. This is the way the model definition has been applied in versions of ASReml prior to Release 4

1. IID residual errors no residual error term specified

```
2. separable autoregressive spatial model of order 1 (AR1 \times AR1)1 2 0 #1 section, 2 variance terms, 0 G structures
rep rep AR1 .1 #the second 'rep' names the data column for sorting
plot plot AR1 0.1
```
3. an equivalent coding for the  $AR1\times AR1$  model using the dimensions of the factors rather than the factor names

```
1 2 0
3 0 AR1 .1
23 0 AR1 0.1
4. variance heterogeneity among the data observations
3 1 0
23 0 ID #default estimate residual variance for all 3 sections
27 0 ID
20 0 ID
5. default residual variance in a multivariate analysis
1 2 0
0 0 ID #let ASReml count how many data records there are
Trait 0 US * #letting ASReml choose start values
```
### 2.5.1 Two rules for defining the residual error term

There are two rules in defining the residual that require special consideration:

Rule 1 The number of effects in the residual term *must* be equal to the number of data units included in the analysis.

Rule 2 Where a compound model term is specified for the residuals, each combination of levels of the single model terms comprising this term must uniquely identify one unit of the data. For example, in the spatial analysis of a column trial comprising 4 replicates of 24 varieties arranged as a grid of 4 rows by 24 columns (rows are replicates), a first order separable autoregressive spatial variance structure for the residuals can be specified by the consolidated model term  $ar1$  (column). $ar1$  (row), where column and row are the appropriate columns in the data file. However, the number of data units must be the product of the number of levels for row and the number of levels for column; 96 in this case. If this is not the case, or if more than one unit is associated with some row column combination, ASReml will return an error message and it will not be possible to use  $ar1$ (column).ar1(row) for residual error. If there are fewer than 96 units and each row-column combination present is associated with one unit, then Section [1.2.2](#page-16-0) shows how to augment the data by completing the grid to allow an appropriate analysis.

These rules will always be satisfied for a single section of data, that is,  $\mathbf{R}_v = \mathbf{R}_{v_1} = \sigma^2 \mathbf{I}_n$ , see Example [2.2,](#page-32-0) defined either by default (ie. with no residual specified) or in terms of the units factor. However, a mismatch in both size and ordering is possible when either multiple sections are present (as in multi-environment trial (MET) analysis) or when non-identity variance model functions are used.

### <span id="page-42-0"></span>2.5.2 Using sat() to specify the residual model term for data with sections

Section [2.3.5](#page-33-0) described partitioning the data observations into data sections to which separate variance structures are applied. There are three data sections in the example variance heterogeneity among the data observations  $(4. \text{ in box on page 34})$ . When variance structures are specified using dimensions rather than factor names ( $idv(23)$  for section 1,  $idv(27)$ ) for section  $2, \ldots$  in the example), the data must be ordered into sections and the variance structures must be ordered to match the order of the sections in the data file. It is usually more convenient to use a variable in the data file to identify sections within the data. The data will be sorted internally by ASReml (ie. the data file does not need to be ordered in any particular way) and the variance structures for sections can then be specified using the sat function, for example

#### residual sat(section).idv(units)

for the simple example with 3 data sections, where section is a new column in the data file to separate the data into the three sections: units  $1 \dots 23$ ,  $24 \dots 50$  and  $51 \dots 70$ . The sat function (shorthand for *section at*) is new with Release 4 and performs several different tasks:

- it tells ASReml that the variance structure for the residual error term is a direct sum structure (see Section [2.3.5\)](#page-33-0) where the different components of the direct sum apply to the different levels of the sectioning variable in the data file
- it prunes the levels for a section so that only the levels of factors defining the residual variance structure for that section are used in forming that variance structure.

Often sections relate to sites (or trials or experiments) in the case where several related trials are analysed together. For example, consider a MET dataset comprising data for three sites. To model the residuals at each site by a separate  $AR1\times ARI$  variance structure, we could write

```
residual sat(site).ar1v(column).ar1(row)
```
Alternatively, an  $AR1\times ARI$  variance structure for sites 1 and 3, but an IDV $\times ARI$  structure for site 2, could be coded using sat either as

```
residual sat(site,1).ar1v(column).ar1(row),
          sat(site,2).idv(column).ar1(row),
          sat(site,3).ar1v(column).ar1(row)
```
or, more succinctly, as

residual sat(site,1,3).ar1v(column).ar1(row) sat(site,2).idv(column).ar1(row)

For each of these definitions, ASReml will determine the particular levels in row and column for each site and hence the appropriate sizes of the AR1 matrices.

Important point A variance structure needs to be specified for every level of the sectioning factor, in which case

residual sat(site,1,3).ar1(row).ar1(column)

would fail as there is no variance structure specified for site 2.

```
3 2 0
row row AR1 .1 #default estimate residual variance for all 3 sections
column column AR1 0.1
row row AR1 .1
column column ID
row row AR1 .1
column column AR1 0.1
```
## <span id="page-43-0"></span>2.6 Identifiability

Once all components of a compound model term have a variance model function applied, ASReml attempts to determine whether the term is identifiable, that is, the terms that can be separately estimated from (are not confounded with) other terms in the model. If the consolidated model term generates a correlation matrix, for example, the consolidated model term for A.B is specified as  $id(A)$ .ar1(B), then it is usually the case that one wishes to fit a model with this correlation structure but to also allow the effects to have a common variance. When a correlation structure is specified for a consolidated term, either for an R or a G structure, ASReml will detect this and add a common scaled variance parameter. Some users might find it simpler and reduce confusion by specifying terms as variance terms directly. For example,  $id(A)$ .ar1(B) should become either  $idv(A)$ .ar1(B) or  $id(A)$ .ar1v(B); it is arbitrary which variable the common variance is attached to. If more than one variance model function in the consolidated model term includes variance parameters, for example  $idv(A)$ .  $ar1v(B)$ , then the parameters will not all be identifiable and so the user must either change  $idv(A)$  to  $id(A)$  and leave  $ar1v(B)$  as it is, or change  $ar1v(B)$  to  $ar1(B)$  and leave  $idv(A)$  as it is.

## <span id="page-44-0"></span>2.7 A sequence of variance structures for the NIN data

Having outlined the theory and introduced the functional specification, we pause now to consider an example. The following is a series of six variance structures of increasing complexity for the NIN column trial data (see Chapter 3 of the User Guide for an introduction to these data). For each example we present a code box to the right that contains the functional specification, a discussion of this code to the left, and the matching code under the structural specification in a code box immediately below. We present the model specification explicitly to help the user understand the logic. In some cases, experienced users will wish to take advantage of reducing typing and clarity by using default rules. These are discussed in Section [2.11.](#page-59-0)

### 1 Randomised complete blocks analysis: blocks fixed

The only random term in a traditional randomised complete block (RCB) analysis of the NIN data is the residual error term  $e \sim$  $N(\mathbf{0}, \sigma_e^2 \mathbf{I}_{224})$ . The model therefore involves just one R structure (IDV) and no G structure. The variance model function name is idv and there is just one consolidated model term; idv(units).



```
NIN Alliance Trial 1989
variety !A
id
...
row 22
column 11
nin89.asd !skip 1
yield ∼ mu variety repl
1 1 0
0 0 ID #default gamma parameterization
```
### 2 RCB analysis: blocks random

The random effects RCB model has 2 random terms to indicate that the total variation in the data is comprised of 2 components; a random replicate term  $u_r \sim N(0, \sigma_r^2 \mathbf{I}_4)$ and the residual error term, as in example 1. The !r before repl tells ASReml that repl is a random term. All random terms must be written after !**r** in the model specification line(s). This model involves both the original IDV R structure and an IDV G structure for the random replicate term. There are now now 2 consolidated model terms; idv(repl) and idv(units).

```
NIN Alliance Trial 1989
variety !A
id
pid
raw
repl 4
.
.
.
row 22
column 11
nin89.asd !skip 1
yield ∼ mu variety,
!r idv(repl)
residual idv(units)
```

```
NIN Alliance Trial 1989
variety !A
id
...
row 22
column 11
nin89.asd !skip 1
yield ∼ mu variety,
!r repl
1 1 0
0 0 ID #default gamma parameterization
```
### 3a Two-dimensional spatial model with spatial correlation in one direction

The NIN trial was actually laid out in as a rectangular array indexed in the data file by row and column. We can therefore consider fitting a spatial model for the residual term where we allow for autocorrelated errors in the row and/or column direction, see Section [2.5.](#page-39-0) However, there are missing plots in the original data. Before fitting a spatial analysis, we therefore need to fill out the data file to contain records for the missing plots. This allows us to define a separable variance structure for the residual error term that is the



kronecker product of a structure for rows and a structure for columns. The example in the code box specifies  $e \sim N(0, \sigma_{e_c}^2 I_{11} \otimes \Sigma_r(\rho_r))$ , that is, a two-dimensional first order separable autoregressive spatial structure for error but with spatial correlation in the row direction only (IDV×AR1): ar1(row) models the  $\Sigma_r(\rho_r)$  correlation structure for rows and idv(column) models the IDV variance structure for columns. The consolidated model term

idv(column).ar1(row)

directly mirrors the algebraic form  $\text{var}(\mathbf{e}) = \sigma_{e_c}^2 \mathbf{I}_{11} \otimes \mathbf{\Sigma}_r(\rho_r)$ .

#### Important points

- the same residual variance structure could be achieved by specifying id(column).ar1v(row) which mirrors the alternate but equivalent algebraic form var  $(e) = I_{11} \otimes \sigma_{e_r}^2 \Sigma_r(\rho_r)$ . It is arbitrary which variable the common variance is attached to: column in the code box, row in the latter, see Section [2.6](#page-43-0) on identifiability.
- if the correlation structure  $id$ (column).ar1(row) was specified, ASReml would automatically add a common variance to model var  $(e) = \sigma_e^2 \mathcal{I}_{11} \otimes \mathcal{I}_{r}(\rho_r)$ , see Section [2.6.](#page-43-0)
- If my is now included in the model specification. This tells ASReml to estimate the missing values. The !f before mv indicates that the missing values are fixed effects in the sparse set of terms. An equivalent way of specifying this model is yield  $∼$  mu variety mv !r idv(repl) where my is the last fixed effect term and ASReml will include my and succeeding terms in the sparse set.
- ASReml would report an error if the consolidated model term  $idv$  (column).ar1v(row) was specified: this would correspond to  $var(e) = \sigma_e^2 \mathbf{I}_{11} \otimes \sigma_{e_r}^2 \mathbf{\Sigma}_r(\rho_r)$  and  $\sigma_e^2$  and  $\sigma_{e_r}^2$  are unidentifiable in this case, that is, it is not possible to estimate them separately.

### 2.7 A sequence of variance structures for the NIN data

• this is a univariate analysis in which case ASReml automatically uses the gamma parameterization for estimation, see Section [2.8.](#page-52-0) Consequently, both the sigmas and the gammas are reported. The user can force ASReml to use the sigma parameterization by placing !SIGMAP immediately after the independent variable and before ∼ on the model definition line:

```
yield !SIGMAP ∼ mu variety mv,
```
!SIGMAP is a new qualifier with Release 4, see also Section [2.8.](#page-52-0) In this case only the sigmas are reported but they appear twice in the output, that is, in both of the columns headed sigma in the .asr file, see Chapter 11 of the User Guide for detailed information on output formats in ASReml.

```
NIN Alliance Trial 1989
variety !A
id
...
row 22
column 11
nin89aug.asd !skip 1
yield ∼ mu variety !r repl !f mv
1 2 0
11 column ID #default gamma parameterization
22 row AR1
```
### 3b Two-dimensional separable autoregressive spatial model

This model extends **3a** by specifying a first order autoregressive correlation structure for columns. The R structure in this case is the kronecker product of two autoregressive correlation matrices, that is, var  $(e) = \sigma_{e_c}^2 \Sigma_c(\rho_c) \otimes$  $\Sigma_r(\rho_r)$ , giving an AR1×AR1 model for error. The consolidated model term in this case is ar1v(column).ar1(row) and includes ar1v(column) to model the  $\sigma_{e_c}^2 \Sigma_c(\rho_c)$  variance structure for columns.

```
NIN Alliance Trial 1989
variety !A
id
.
.
.
row 22
column 11
nin89aug.asd !skip 1
yield ∼ mu variety,
!r idv(repl) !f mv
residual ar1v(column).ar1(row)
```
#### Important points

- the same residual variance structure could be achieved by specifying  $ar1$ (column). $ar1v$ (row) which mirrors the alternate but equivalent algebraic form  $\text{var}(\boldsymbol{e}) = \boldsymbol{\Sigma}_c(\rho_c) \otimes \sigma_{e_r}^2 \boldsymbol{\Sigma}_r(\rho_r).$
- if the correlation structure  $ar1$ (column). $ar1$ (row) was specified, ASReml would automatically add a common variance, see Section [2.6.](#page-43-0)
- ASReml would report an error if the consolidated model term  $ariv$  (column). $ariv$  (row) was specified as this would correspond to var  $(e) = \sigma_{e_c}^2 \Sigma_c(\rho_c) \otimes \sigma_{e_r}^2 \Sigma_r(\rho_r)$  and  $\sigma_{e_c}^2$  and  $\sigma_{e_r}^2$ are unidentifiable, that is, it is not possible to estimate them separately, see Section [2.6.](#page-43-0)

```
NIN Alliance Trial 1989
variety !A
id
...
row 22
column 11
nin89aug.asd !skip 1
yield ∼ mu variety !r repl !f mv
1 2 0
11 column AR1 #default gamma parameterization
22 row AR1
```
## 3c Two-dimensional separable autoregressive spatial model with measurement error

This model extends 3b by adding a random units term. Thus

 $\text{var}\left(\bm{u}_{r}\right)=\sigma_{r}^{2}\bm{I}_{4}$ ,  $\text{var}\left(\bm{u}_{\eta}\right)=\sigma_{\eta}^{2}\bm{I}_{_{242}}$  and var  $(e) = \sigma_{e_c}^2 \Sigma_c(\rho_c) \otimes \Sigma_r(\rho_r)$ . The reserved word units tells ASReml to construct an additional random term with one level for each experimental unit, so that a second (independent) error term can be fitted. A units term is fitted in the model in cases like this where a variance structure is applied to the errors. An



IDV variance structure is specified for units to model  $\sigma_{\eta}^2 I_{242}$ . The units term is sometimes fitted in spatial models for field trial data to allow for a nugget effect. The model now has two terms at the plot (experimental unit) level, that is, a correlated structure defined as an R structure and an uncorrelated structure defined in the G structure. There are now three consolidated model terms;  $idv(repl)$ ,  $idv(units)$  and  $arlv(colum)$ .  $ar1(row)$ . This order is reversed in 4.

```
NIN Alliance Trial 1989
variety !A
id
...
row 22
column 11
nin89aug.asd !skip 1
yield ∼ mu variety !r repl units !f mv
1 2 0
11 column AR1 #default gamma parameterization
22 row AR1
```
## 4 Two-dimensional separable autoregressive spatial model defined as a G structure

This model is equivalent to 3c but with the spatial model defined as a G structure rather than an R structure. The algebraic form is written alternatively, but equivalently, to the form in 3c, that is  $\text{var}\left(\boldsymbol{u}_{r}\right)=\sigma_{r}^{2}\boldsymbol{I}_{4},$ var  $(\boldsymbol{u}_{cr}) = \sigma_{cr_c}^2 \boldsymbol{\Sigma}_c(\rho_c) \otimes \boldsymbol{\Sigma}_r(\rho_r)$  and

#### NIN Alliance Trial 1989 variety !A id . . . row 22 column 11 nin89aug.asd !skip 1 yield ∼ mu variety, !r idv(repl) ar1v(column).ar1(row) !f mv residual idv(units)

#### Important points

 $var(\bm{e}) = \sigma_e^2 \; I_{242}.$ 

- the same G structure could be achieved by specifying  $ar1$  (column).  $ar1v$  (row), see similar comment in example 3b
- if the variance structure  $ariv$  (column).  $ariv$  (row) was specified ASReml would report an error, see identical comment in example 3b
- estimation is based on the gamma parameterization in which case both the estimated sigmas and the estimated gammas are reported. The user can force ASReml to use the sigma parameterization by placing the !SIGMAP qualifier immediately after the independent variable and before ∼ on the model definition line. In this case only the sigmas would be reported, but they would be repeated in the column headed gamma in the output, see Important points under example 3a.

```
NIN Alliance Trial 1989
variety !A
id
...
row 22
column 11
nin89aug.asd !skip 1
yield ∼ mu variety !r repl mu.column.row !f mv
1 1 1
0 0 ID #default gamma parameterization
```
## <span id="page-52-0"></span>2.8 Sigma versus gamma parameterization

From Section [2.3.1,](#page-31-0) the variance matrix of  $y$  is

 $\text{var}\left(\boldsymbol{y}\right) \;\;=\;\; \boldsymbol{Z}\boldsymbol{G}(\boldsymbol{\sigma}_g)\boldsymbol{Z}^{\intercal}+\boldsymbol{R}_v(\boldsymbol{\sigma}_r),$ 

see model [\(2.3\)](#page-31-1). This is referred to as the sigma parameterization and the individual variance structure parameters in  $\sigma_q$  and  $\sigma_r$  are referred to as *sigmas*. For the case when the variance structure for the residual error term is a scaled correlation matrix, that is,  $\bm{R}_v(\bm{\sigma}_r) = \sigma_e^2 \bm{R}_c(\bm{\gamma}_r)$ , the variance matrix of  $\bm{y}$  can be written alternatively as

$$
\text{var}\left(\boldsymbol{y}\right) \;\; = \;\; \sigma_e^2\left(\boldsymbol{Z}\boldsymbol{G}(\boldsymbol{\gamma}_g)\boldsymbol{Z}^\intercal + \boldsymbol{R}_c(\boldsymbol{\gamma}_r)\right),
$$

see [\(2.8\)](#page-34-0). This is referred to as the gamma parameterization and the variance structure parameters in  $\gamma_q$  and  $\gamma_r$  are referred to as gammas, see Section [2.3.6.](#page-33-1)

### 2.8.1 Which parameterization does ASReml use for estimation?

ASReml switches between the sigma and the gamma parameterizations depending on the residual model specification. The current default for univariate, single section data-sets is the gamma parameterization. It is possible to over-ride this default as discussed in the following section. ASReml reports both the gammas and the sigmas when the gamma parameterization is used for estimation. For historical reasons, the sigmas are presented twice (two identical columns) when the sigma parameterization is used for estimation.

ASReml uses the sigma parameterization for analyses other than univariate and/or single site analyses, examples including multi-section analyses, multivariate analyses and repeated measures analysis using R structures that are not the default variance model (ie. scaled identity).

#### 2.8.2 Switching from the gamma to the sigma parameterization

ASReml uses the gamma parameterization by default for univariate and/or single section analyses, see above. However, !SIGMAP is a new qualifier with Release 4 that enables the user to force ASReml to use the sigma parameterization this case. This is achieved by placing !SIGMAP immediately after the independent variable and before ∼ on the model definition line. For example,

yield !SIGMAP ∼ mu variety !r idv(repl) !f mv residual idv(units)

would force ASReml to use the sigma parameterization in NIN example 3a, see Section [2.7.](#page-44-0)

Table [2.3](#page-53-0) gives the variance model specification for each of the six NIN examples (column 3), the individual terms in  $G(\sigma_q)$  and  $R_v(\sigma_r)$  under the sigma parameterization (column 4), the sigmas that are estimated under this parameterization (column 5), the individual terms in  $G(\gamma_g)$  and  $\mathbf{R}_v(\gamma_r)$  under the gamma parameterization (column 6) and the gammas that are estimated under this parameterization (column 7).

<span id="page-53-0"></span>

## 2.9 Variance model functions available in ASReml

The full range of variance models, that is, correlation, homogeneous variance and heterogeneous variance models available in ASReml is presented in Table [2.5](#page-61-0) which is located at the end of this document for easy access, see Section [2.12](#page-61-1) on page [54.](#page-61-1) This presents the variance structure name (in UPPERCASE), the corresponding variance model function name (in lowercase) used to associate the variance structure with the appropriate component of a model term, a brief description, the algebraic form of the model and the number of associated variance structure parameters.

The models span correlation (base) models (diagonal elements equal to 1 and correlations on the off diagonals), the extension of these to variance models (variances on the diagonals and covariance on the off diagonals), additional models that are parameterized as variance matrices rather than as correlation matrices and some special cases where the covariance structure is known except for the scale.

### 2.9.1 Forming variance models from correlation models

The variance function models presented under correlation models in Table [2.5](#page-61-0) (id ... matk) are used to specify the correlation models for the corresponding variance structures. The corresponding homogeneous and heterogeneous variance models are specified by appending v and h to the variance model function names respectively, and appending the corresponding variance parameters to the corresponding list of parameters. This convention holds for most models. It does not make sense to append v or h to the variance model function names for the heterogeneous variance models from diag  $\dots$  xfak.

In summary:

• to specify a correlation model, provide the variance model function name given in Table [2.5,](#page-61-0) for example, for a factor row

#### exp(row)

is an exponential correlation model with a single correlation parameter,

• to specify an homogeneous variance model, append a v to the variance model function name, for example

expv(row)

is an exponential variance model with 2 parameters (correlation and variance),

• to specify a heterogeneous variance model, append an h to the variance model function name, for example

coruh(site)

is a variance matrix with different variances for each site but the same correlation for all pairs of sites.

Important See Section [2.6](#page-43-0) for rules on combining variance models and Section [2.10.1](#page-56-0) for important notes regarding initial values.

## <span id="page-55-0"></span>2.10 New variance model function qualifiers

A consolidated model term is comprised of one or more covariance components, where a covariance component is a component of the model term to which a variance model function has been applied, see Section [2.4](#page-34-1) and Table [2.1.](#page-36-0) All of the covariance components so far have been of the form

vmfname(component)

where *vmfname* is the variance model function name (in this font in first column of Table [2.5\)](#page-61-0) and component is a component in the model term. Two single covariance components are  $idv$ (repl) and  $ar1(row)$ , see Table [2.1.](#page-36-0)

A general form for a covariance component is

vmfname(single component qualifiers)

where *qualifiers* is an optional list of one or more qualifiers to be applied to the variance structure being defined. A simple example of this is the extension of  $\text{idx}(\text{rep1})$  to  $\text{idx}(\text{rep1})$ !INIT 0.65) which specifies an IDV structure of dimension 4 for replicates (NIN example 2) with an initial variance of 0.65 for the variance component associated with replicates under the sigma parameterization, or an initial variance component ratio of 0.65 for the variance component ratio associated with replicates under the gamma parameterization.

Note that a variance structure of a particular dimension,  $\omega$  say, can been specified directly as

 $vminame(\omega$  qualifiers)

For example,  $i \text{dv}(3)$  defines the IDV variance structure of dimension 3, that is,  $\sigma^2 I_3$ , and idv(3 !INIT 1.1) specifies an initial value of 1.1 for the associated variance component under the sigma parameterization or variance ratio under the gamma parameterization. Likewise,  $ar1(10)$  specifies an autoregressive correlation structure (AR1) of order 10 and ar1(10 !INIT 0.4) specifies this same structure with an initial autocorrelation parameter of 0.4. A simple variance component  $\sigma^2$  would be defined as  $i \frac{dv(1)}{dt}$ . Note that an integer value for the first argument is only valid in variance model functions associated with residual terms and str().

New qualifiers are in Table [2.4](#page-56-1) (see Section 7.7 of the User Guide for the full list of qualifiers).

#### 2.10 New variance model function qualifiers

In the structural specification the G structure is specified on G structure lines placed after any R structure lines. There must be a variance header line immediately after the model line. It specifies three numbers,  $s, c$  an  $q$ .  $s$  and  $c$  relate to the R structure and are defined on page [34.](#page-39-0) g is the number of (random) model terms which have a variance structure explicitly defined as described here. Each specification begins with a G structure header line. It contains the name of the model term and the number of components. For each component, the variance structure is then specified, nominating the

size key structure initial-parameter-values qualifiers where

size is the name of the component or the number of effects in it

key is 0 for most G structure cases

structure is the name of variance structure

initial-parameter-values and qualifiers are discussed later.

<span id="page-56-1"></span>In the structural specification it is not now mandatory to specify initial values.



#### Table 2.4: New variance model function qualifiers available in ASReml

For existing qualifiers, please refer to Chapter 7 in ASReml User Guide Release 4, Functional Specification.

### <span id="page-56-0"></span>2.10.1 Initial values ! INIT  $v$

Prior to Release 4 it was necessary to supply initial values for variance structure parameters except for the default IDV variance structure for a random model term, where the default initial variance (ratio) parameter value was 0.1. In Release 4, it is not generally necessary to supply initial values. In this release, ASReml provides starting or initial values for variance structure parameters based on knowledge of the phenotypic variance of the response. Occasionally these initial values are not adequate and more appropriate values will need to be supplied by the user. In this case the user may have good prior information that can be utilized in forming initial values.

There are several ways to provide initial values. The particular choice will depend on how

many values and other variance model function qualifiers are to be specified. The initial values can be provided in a number of ways:

• in the variance structure specification, for example

```
ar1(row !INIT 0.35)
```
sets the initial value of the autocorrelation parameter for  $ar1(row)$  at 0.35; when this form is used, all of the values required by the structure must be specified

- by modifying the .tsv or .msv file created in a preliminary run (Section [1.1.2\)](#page-9-0)
- by supplying an .rsv file using !CONTINUE, refer to the User Guide.

#### Important points

- when initial values are supplied using !INIT, there must be the correct number of values and they must be in the appropriate order, for example, for us() the initial values need to be supplied in the order lower triangle row-wise
- for the gamma parameterization (Section [2.8\)](#page-52-0), the variance structure parameters will be gammas; in this case the initial values for the gammas that are variance component ratios will be interpreted by ASReml as ratios.

The qualifiers are the same as for the structural specification except that:

- they are specified on the R and G structure lines in the structural specification, see (see pages [49](#page-55-0) and [34\)](#page-39-0)
- the !INIT qualifier name is not defined in the structural formulation because initial values are always expected
- the !COORD qualifier was not provided in the structural specification: if v was required, it was supplied as an unadorned vector after the G structure lines.

### <span id="page-57-0"></span>2.10.2 Ways to supply distances in one-dimensional metric based models  $! \text{COPBD}$  v

Power models rely on the definition of distance for the associated term. Information for determining distances is supplied either implicitly by applying the variance model function to the fac() of the coordinate variables, for example

expv(fac(X))

where X contains the positions, or explicitly with the **!COORD** qualifier, for example

 $\exp$ v(Time !COORD  $x$ )

<span id="page-58-0"></span>where  $x$  is a vector of distances which has to be of length the number of levels of Time.

### 2.10.3 About subsections ! SUBSECTION f

The !SUBSECTION qualifier provides an extension to the sat function of Section [2.5.2](#page-42-0) for modelling the residual variance. It allows the case of modelling multiple independent sections of correlated observations with a common variance structure and common parameters within sections. The sections can be of different sizes and any homogeneous variance correlation model in Table [2.5](#page-61-0) may be used for the variance structure. This gives an R structure of the form

$$
\boldsymbol{R}_v = \oplus_{i=1}^s \boldsymbol{R}_{v_i} \quad \text{where} \quad \boldsymbol{R}_{v_i} = \oplus_{j=1}^{s_i} \boldsymbol{\Sigma}_{ij}(\boldsymbol{\phi}_i)
$$

so  $\mathbf{R}_{v_i}$  may have a direct sum structure with common parameters. Note that, !SUBSECTION is only available when the residual variance function is expressed in terms of one variance function. !SUBSECTION  $f$  performs two tasks similar to those described in Section [2.5.2,](#page-42-0) that is, defining a direct sum structure for the residual vector in a section, with the number of subsections in section i,  $s_i$ , given by the number of levels of the factor f, and pruning the levels of the factor defining the variance structure within each section but allowing common variance parameters across sections. The data needs to be sorted in order of the variable f. The following code would specify a common AR1 structure across sections, assumed sorted in to the appropriate order within the section variable, with an initial spatial autocorrelation parameter of 0.5

residual ar1(units !INIT 0.5 !SUBSECTION section)

If there was data sorted on date within plot then we might use

residual exp(date !INIT 0.2 !SUBSECTION plot)

<span id="page-58-1"></span>to, specify a common EXP structure across plots.

### 2.10.4 Equating variance structures ! USE  $t$

In some plant breeding applications, it can be convenient to define a variance structure as the sum of two simpler terms. For example, given 1000 entries representing 50 related families, where relationships were derived from markers, the full relationship matrix (inverse) is dense. But it can be well approximated as the sum of a family component and a diagonal entry component. The reformulation gives a sparser (faster) formulation. But now we have two terms to interact with  $xfa1(dtrial)$  and both must have the same parameters. That is, instead of fitting

```
xfa1(dTrial).grm3(entry)
we fit
xfa1(dTrial).grm1(family) xfa1(dTrial).grm2(entry)
requiring both xfa1 terms have the same parameters.
```
If there are only a few parameters, this can be achieved directly as follows:

```
!ASSIGN QP !GPFPFP
!ASSIGN QE !=%ABCDEFGH
!ASSIGN QI !INIT 0.72631 0.000 .242713 0.000 .882465 .846305 .04419 .743393
xfa1(dTrial).grm1(family $QP $QE $QI),
xfa1(dTrial).grm2(entry $QP $QE $QI)
```
However, for a larger term, the number of parameters required may exceed the available letters in the alphabet. In this case !VCC can be used:

```
<DATAFILE NAME> !VCC 1
...
xfa1(dTrial).grm1(family $QP $QI),
xfa1(dTrial).grm2(entry) $QP $QI)
21 29 !BLOCKSIZE 8 #parameters 21:28 are equal to parameters 29:36 pairwise
```
An ever better option in this case is to use just one structure twice. The following code associates xfa1(dTrial) in xfa1(dTrial).giv2(entry) with xfa1(dTrial) in xfa1(dTrial).giv1(family) , that is, both terms point to the one structure definition:

```
xfa1(dTrial).grm1(family $QP $QI)
xfa1(dTrial !USE xfa1(dTrial)).grm2(entry)
```
## <span id="page-59-0"></span>2.11 Default variance structures in ASReml

There are default variance structures in ASReml that allow the linear mixed model to be specified more succinctly. IDV is the default variance structure for random model terms and for the residual error terms. For example

- A will be interpreted as  $idv(A)$
- $A.B$  will be interpreted as  $idy(A.B)$
- A.B.C will be interpreted as idv(A.B.C)
- sat(Expt, 1). A will be interpreted as  $sat(Expt,1).idx(A)$
- sat(Expt,1).A.B will be interpreted as sat(Expt,1).idv(A.B)
- sat(Expt,1).A.B.C will be interpreted as sat(Expt,1).idv(A.B.C)

In these cases the model term can be followed by an initial value and/or a parametric qualifier for example A 1 !GP is interpreted as idv(A !INIT 1 !GP) there is always a residual error term in the model but if it is not explicitly specified it is assumed to be idv(units). If the consolidated model term definition is incomplete, that is, if some but not all of the

components have a variance model function specified, the variance model functions idv() or id() will be applied to these components depending on the variance model functions specified. For example

- $idv(A)$ .B will be interpreted as  $idv(A)$ . $id(B)$
- $id(A)$ .B will be interpreted as  $id(A)$ . $idv(B)$
- $id(A)$ .B.C will be interpreted as  $id(A)$ . $idv(B.C)$
- $idv(A)$ .B.C will be interpreted as  $idv(A)$ . $id(B.C)$

Similarly, at the residual level as sat() cannot be converted into a variance function

- $-$  sat(Expt, 1).id(A).B will be interpreted as sat(Expt, 1).id(A).idv(B)
- sat(Expt,1).id(A).B.C will be interpreted as sat(Expt,1).id(A).idv(B.C)
- $-$  sat(Expt, 1).idv(A).B.C will be interpreted as sat(Expt, 1).idv(A).id(B.C)

However, it is good practice to specify variance model functions for the components in model terms and we encourage the user to do this. ASReml will automatically add a common variance to consolidated model terms that are specified as correlation models for both R and G structures, for example,

- $id(A)$  will be converted to  $idv(A)$
- sat(Expt,1).id(units) will be converted to sat(Expt,1).idv(units)
- $id(A) . ar1(B)$  will be converted to  $idv(A) . ar1(B)$
- $-$  ar1(A).ar1(B) will be converted to  $ar1v(A)$ .ar1(B)
- sat(Expt,1).id(A).ar1(B) will be converted to sat(Expt,1).idv(A).ar1(B)
- sat(Expt, 1).ar1(A).ar1(B) will be converted to sat(Expt, 1).ar1 $v(A)$ .ar1(B)

Using NIN example 2 for demonstration (Section [2.7\)](#page-44-0), a more succinct coding of the model definition would be

yield ∼ mu variety !r repl residual units

which would result in identical output to the original example. The model could be relaxed further to

yield ∼ mu variety !r repl

## <span id="page-61-1"></span>2.12 Variance models available in ASReml

Table 2.5: Details of the variance models available in ASReml

<span id="page-61-0"></span>

## correlation models

#### One-dimensional, equally spaced







 $0 < \phi < 1$ 



## heterogeneous variance models





GRM8 grm8



Details of the variance models available in ASReml

<sup>†</sup> This is the number of variance structure parameters,  $\omega$  is the dimension of the matrix. The homogeneous variance form is specified by appending V to the correlation basename; the heterogeneous variance form is specified by appending H to the correlation basename

generalized relationship matrix  $8 \t 0 \t 1$ 

‡ These will be associated with 1 variance parameter unless used in direct product with another structure that provides the variance. Appending a v to a name makes it explicit that a variance parameter is fitted.

## 2.13 Functions of variance components using names

Rather than identifying parameters by number when specifying functions in VPREDICT ASReml4 allows parameters to be named. When ASReml reads back the variance parameters from the .asr file, each covariance component, or variance function, is assigned a name. The functional specification allows a more explicit naming convention than the structural specification. The full name is usually the covariance function, or its specified contracted form, prepended by the consolidated model term, or its specified contracted form, and the symbol ;. Exceptions to this rule are single components F,  $id[v](F)$  and  $nrm[v](F)$  terms which are reduced to the corresponding single term  $F$ ,  $id[v](F)$  and  $nrm[v](F)$ . So, for example, with the random model and residual specification model terms

```
!r idv(A) ar1v(B) nrm(C).us(Trait) D residual id(units).us(Trait)
The covariance functions with parameters
idv(A), artv(B), us(Train) in nrm(C).us(Train)and
```
us(Trait) in id(units).us(Trait) are named

 $idv(A), ar1v(B); ar1v(B), nrm(C).us(Trait);us(Trait), id(units).us(Trait);us(Trait).$ If the resulting name is not ambiguous the name can be contracted by reducing the consolidated model term to a unique substring or leaving out the consolidated model term completely. For example, in the example the covariance functions can be represented by idv(A), ar1v(B), C;us(Trait) and units;us(Trait), respectively. Individual parameters within a covariance component can be specified by number, or sequence of numbers  $(n : m)$  by appending these in square braces, for example, C;us(Trait)[3] or units;us(Trait)[4:6]. If the residual directive is not used, the default R structure parameters are effectively named Residual.

### 2.13.1 A detailed example

The following example for a **bivariate sire model** is a little more complicated. The job file bsiremod.as contains

... coop.fmt ywt fat ~ Trait Trait.(age c(brr) sex sex.age) !r us(Trait).id(sire);us(Trait) !f Tr.grp residual id(units).us(Trait) VPREDICT !DEFINE F phenvar id(units).us(Trait);us(Trait) + us(Trait).sire;us(Trait) # 1:3 + 4:6 F addvar sire:us(Trait) \* 4 F addvar sire;us(Trait) \* 4 <br>
H heritA addvar[1] phenvar[1] <br>
# 10 7 <br>
# 10 7  $H$  heritA addvar[1] phenvar[1] H heritB addvar[3] phenvar[3]  $\qquad$  # 12 9<br>R phencorr phenvar  $\qquad$  # 7 8 9

The relevant lines of the .asr file are

R phencorr phenvar



R gencorr addvar  $#4:6$ 

Numbering the parameters reported in bsiremod.asr (and bsiremod.vvp)

```
1
     error variance for ywt
```
- 2 error covariance for ywt and fat
- 3 error variance for fat
- 4 sire variance component for ywt
- 5 sire covariance for ywt and fat
- 6 sire variance for fat

then

```
F phenvar id(units).us(Trait);us(Trait) + us(Trait).id(sire);us(Trait) or
```


The resulting .pvc file contains:



The first 8 lines are based on the  $\,.\, {\tt asr}$  file.

# 3 Examples

This chapter takes examples from the User Guide and compares the functional specification to the structural specification. Please refer to the User Guide for a comprehensive description of each dataset and analysis.

Throughout this chapter, this font and colour are used for code that is common to both specifications. The first three examples [\(3.1](#page-69-0) to [3.3\)](#page-70-0) involve uncorrelated G and R structures, that is, the IDV variance structure for both the random model terms and the residual error term. As such, the explicit functional specification can be simplified to the structural specification. In these examples, this font and colour are used for STRUCTURAL AND IMPLICIT FUNCTIONAL code and this font and colour are used for EXPLICIT FUNCTIONAL code. In the remaining examples (from [3.4\)](#page-71-0), this font and colour are used for STRUCTURAL code and this font and colour are used for FUNCTIONAL code. Note that, these examples present two alternative model specifications. To run the jobs retaining both model specifications in the command file, one of the specifications could be commented out.

## <span id="page-69-0"></span>3.1 Split plot design - Oats

```
split plot example
blocks 6 #coded 1...6 in first data field of oats.asd
nitrogen !A 4 #coded alphabetically
subplots * #coded 1...4
variety !A 3 #coded alphabetically
wplots * #coded 1...3
yield
oats.asd !SKIP 2
#STRUCTURAL and IMPLICIT FUNCTIONAL
yield ∼ mu variety nitrogen variety.nitrogen !r blocks blocks.wplots
#EXPLICIT FUNCTIONAL
yield ∼ mu variety nitrogen variety.nitrogen !r idv( blocks) idv(blocks.wplots)
residual idv(units)
```
## 3.2 Unbalanced nested design - Rats

```
Rats example
dose 3 !A
sex 2 !A
littersize
dam 27
pup 18
weight
rats.asd !DOPATH 1 #change DOPATH argument to select each PATH
!PATH 1
#STRUCTURAL AND IMPLICIT FUNCTIONAL
weight ∼ mu littersize dose sex dose.sex !r dam
#EXPLICIT FUNCTIONAL
weight ∼ mu littersize dose sex dose.sex !r idv(dam)
residual idv(units)
!PATH 2
#STRUCTURAL AND IMPLICIT FUNCTIONAL
weight ∼ mu out(66) littersize dose sex dose.sex !r dam
#EXPLICIT FUNCTIONAL
weight ∼ mu out(66) littersize dose sex dose.sex !r idv(dam)
residual idv(units)
!PATH 3
#STRUCTURAL AND IMPLICIT FUNCTIONAL
weight ∼ mu littersize dose sex !r dam
#EXPLICIT FUNCTIONAL
weight ∼ mu littersize dose sex !r idv(dam)
residual idv(units)
!PATH 4
#STRUCTURAL AND IMPLICIT FUNCTIONAL
Weight ∼ mu littersize dose sex
#EXPLICIT FUNCTIONAL
weight ∼ mu littersize dose sex
residual idv(units)
```
## <span id="page-70-0"></span>3.3 Source of variability in unbalanced data - Volts

```
Voltage data
teststat 4 #4 testing stations tested each regulator
setstat !A #10 setting stations each set 4-8 regulators
regulator 8 #regulators numbered within setting stations
voltage
voltage.asd !skip 1
#STRUCTURAL AND IMPLICIT FUNCTIONAL
voltage ∼ mu !r setstat setstat.regulator teststat setstat.teststat
```

```
#EXPLICIT FUNCTIONAL
voltage ∼ mu !r idv(setstat) idv(setstat.regulator) idv(teststat),
idv(setstat.teststat)
residual idv(units)
```
<span id="page-71-0"></span>The next three examples gives examples of different residual structures.

## 3.4 Balanced repeated measures - Height

```
This is plant data multivariate
tmt !A #diseased Healthy
plant 14
y1 y3 y5 y7 y10
grass.asd !skip 1 !ASUV
!Y y1 !G tmt !JOIN #plot the data
```
First a split plot in time model can be fitted by fitting a units term plus an independent residual.

```
#STRUCTURAL
y1 y3 y5 y7 y10 ∼ Trait tmt Trait.tmt !r units
1 2 0 #1 section 2 dimensions 0 G structure
14 0 ID #14 units no reordering ID structure can reduce to 14
Trait 0 ID
#FUNCTIONAL
y1 y3 y5 y7 y10 ∼ Trait tmt Trait.tmt !r idv(units)
residual idv(units.Trait)
```
Next a split plot in time model can be fitted by specifying a CORU variance model for the R structure

```
#STRUCTURAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
1 2 0
14Trait 0 CORU .5
#FUNCTIONAL
y1 y3 y5 y7 y10 ∼ Trait tmt Trait.tmt
residual idv(units).coru(Trait)
```
Next an exponential (EXP) model to allow the correlation between observations to decline with time differences.

```
#STRUCTURAL
y1 y3 y5 y7 y10 ∼ Trait tmt Trait.tmt
1 2 0
14
Trait 0 EXP .5
```
```
1 3 5 7 10 #time coordinates
#FUNCTIONAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
residual id(units).exp(Trait !INIT 0.5 !COORD 1 3 5 7 10)
Next an exponential model with heterogeneous variances (EXPH) is fitted
#STRUCTURAL
y1 y3 y5 y7 y10 ∼ Trait tmt Trait.tmt
1 2 0
14 !S2==1
Trait 0 EXPH .5 100 200 300 300 300
1 3 5 7 10
#FUNCTIONAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
residual id(units).exph(Trait !INIT 0.5 100 200 300 300 300 !COORD 1 3 5 7 10 )
Next an antedependence model with heterogeneous variances (EXPH) is fitted
!ASSIGN ANTE1 !< !INIT 60.16
54.65 73.65
91.50 123.3 306.4
89.17 120.2 298.6 431.8
62.21 83.85 208.3 301.2 379.8 !>
#ASSIGN used to make input more legible
residual units.ante(Trait !INIT $ANTE1)
#STRUCTURAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
1 2 0
14 !S2==1
Trait 0 ANTE $ANTE1
#FUNCTIONAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
residual idv(units).ante(Trait !INIT $ANTE1)
Finally, an unstructured (US) matrix is fitted.
!ASSIGN US1 !< !INIT 37.20
23.38 41.55
34.83 61.89 258.9
44.58 79.22 331.4 550.8
43.14 76.67 320.7 533.0 541.4 !>
#STRUCTURAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
1 2 0
14 !S2==1
Trait 0 US $US1
#FUNCTIONAL
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
```
residual id(units).us(Trait !INIT \$US1)

An alternative way of fitting an unstructured error model for multivariate data is to omit the !ASUV qualifier. #STRUCTURAL

```
y1 y3 y5 y7 y10 \sim Trait tmt Trait.tmt
1 2 0
\OmegaTrait 0 US * #ASReml generates initial values
#FUNCTIONAL
y1 y3 y5 y7 y10 ∼ Trait tmt Trait.tmt
residual id(units).us(Trait) #ASReml generates initial values
```
#### 3.5 Spatial analysis of a field experiment - Barley

```
!EPS !RENAME !ARG 1 2 3
Slate Hall example
Rep 6 #six replicates of 5x5 plots in 2x3 arrangement
RowBlk 30 #rows within replicates numbered across replicates
ColBlk 30 #columns within replicates numbered across replicates
row 10 #field row
column 15 #field column
variety 25
yield
barley.asd !skip 1 !DOPATH $1
!PATH 1 #AR1 x AR1
#STRUCTURAL
y ∼ mu var
1 2
15 column AR1 0.1 #second field is specified so ASReml can sort
10 row AR1 0.1 #records properly into field order
#FUNCTIONAL
y ∼ mu var
residual ar1v(column).ar1(row)
!PATH 2 #AR1 x AR1 + units
#STRUCTURAL
y ∼ mu var !r units
1<sub>2</sub>15 column AR1 0.1
10 row AR1 0.1
#FUNCTIONAL
y ∼ mu var !r idv(units)
residual ar1v(column).ar1(row)
!PATH 3 #incomplete blocks
#STRUCTURAL
y ∼ mu var !r Rep Rowblk Colblk
```

```
#FUNCTIONAL
y ∼ mu var !r idv(Rep) idv(Rowblk) idv(Colblk)
residual idv(units)
```
## 3.6 Unreplicated early generation variety trial - Wheat

```
!EPS !RENAME !ARG 1 2 3 4
Tullibigeal Trial !DOPART $1
linenum
yield
weed
column 10
row 67
variety 532 #testlines 1:525, check lines 526:532
wheat.asd !SKIP 1
#AR1 x ID
!PART 1
#STRUCTURAL
y ∼ mu weed mv !r variety
1 2 0
67 row AR1 0.1
10 column ID
#FUNCTIONAL
y ∼ mu weed mv !r idv(variety)
residual ar1v(row).id(col)
#AR1 x AR1
!PATH 2
#STRUCTURAL
y ∼ mu weed mv !r variety
1 2 0
67 row AR1 0.1
10 column AR1 0.1
#FUNCTIONAL
y ∼ mu weed mv !r variety
residual ar1v(row).ar1(col)
!PATH 3 #AR1 x AR1 + column trend
#STRUCTURAL
y ∼ mu weed pol(column,-1) mv !r variety
1 2 0
67 row AR1 0.1
10 column AR1 0.1
#FUNCTIONAL
y ∼ mu weed pol(column,-1) mv !r variety
residual ar1v(row).ar1(col)
!PATH 4 #AR1 x AR1 + nugget + column trend
#STRUCTURAL
```

```
y ∼ mu weed pol(column,-1) mv !r variety units
1 2 0
67 row AR1 0.1
10 column AR1 0.1
#FUNCTIONAL
y ∼ mu weed pol(column,-1) mv !r variety units
residual ar1v(row).ar1(col)
```
## 3.7 Paired Case-Control study - Rice

This includes 3 analyses, one using uncorrelated effects, the second allowing heterogeneous variances to some effects, and thirdly a bivariate analysis. The data for the first two analyses is in file rice.asd and the data for the third analysis is in ricem.asd. The input for the first two analyses is:

```
Bloodworm data Dr M Stevens
pair 132
rootwt
run 66
tmt 2 !A
id
variety 44 !A
rice.asd !skip 1
!DOPATH 1 #change to 2 for second analysis
!PATH 1
#STRUCTURAL AND IMPLICIT FUNCTIONAL
sqrt(rootwt) ∼ mu tmt !r variety variety.tmt run pair run.tmt
#EXPLICIT FUNCTIONAL
sqrt(rootwt) ∼ mu tmt !r idv(variety) idv(variety.tmt) idv(run),
idv(pair) idv(run.tmt)
residual idv(units)
!PATH 2
#STRUCTURAL
sqrt(rootwt) ~ mu tmt !r variety tmt.variety run pair,
tmt.run uni(tmt,2)
0 0 2
tmt.variety 2
2 0 DIAG .1 .1 !GU
44 0 0
tmt.run 2
2 0 DIAG .1 .1 !GU
66 0 0
#FUNCTIONAL
sqrt(rootwt) ∼ mu tmt !r idv(variety) diag(tmt).idv(variety) idv(run) idv(pair),
diag(tmt).id(run) uni(tmt,2)
residual idv(units)
```
#### 3.8 Balanced longitudinal data - Random coefficients and cubic smoothing splines - **Oranges**

The input for the third analysis is

```
id
 pair 132
 run 66
 variety 44 !A
 yc #Control tray
 ye #Treated tray
ricem.asd !skip 1
!X yc !Y ye
tabulate sqrt(yc) sqrt(ye) \sim var run !COUNT
#STRUCTURAL
sqrt(yc) sqrt(ye) ∼ Trait !r Trait.variety Trait.run
1 2 2
132 !S2==1
Trait 0 US 2.21 1.1 2.427
Trait.variety 2
2 0 US 1.401 1 1.477
44 0 0
Trait.run 2
2 0 US .79 .5 2.887
66 0 0
PREDICT variety
#FUNCTIONAL
sqrt(yc) sqrt(ye) ~ Trait !r us(Trait).id(variety) us(Trait).id(run)
residual id(units).us(Trait)
PREDICT variety
```
# 3.8 Balanced longitudinal data - Random coefficients and cubic smoothing splines - Oranges

This includes initial analyses on one tree,random coefficient effect and smoothing splines models !RENAME !ARG 1 #First analysis: replace with 2 for next analysis !DOPART \$1 this is the orange data, seq #record number is not used tree 5 age #118 484 664 1004 1231 1372 1582 circ season !L Spring Autumn !PART 1 #INDIVIDUAL TREE orange.asd !skip 1 !filter tree !select 1 !PART 2 orange.asd !skip 1 !PART 0

```
!SPLINE spl(age,7) 118 484 664 1004 1231 1372 1582
!PVAL age 150 200:1500
!PATH 1
#STRUCTURAL AND IMPLICIT FUNCTIONAL
circ ∼ mu age !r spl(age,7)
#EXPLICIT FUNCTIONAL
circ ∼ mu age !r idv(spl(age,7))
residual idv(units)
!PATH 2
#STRUCTURAL
circ ∼ mu age !r !{tree 4.6 age.tree .000094!} spl(age,7) .1,
spl(age,7).tree 2.3 fac(age) 13.9
0 0 1
tree 2
2 0 US 4.6 .00001 .000094
5 0 0
#FUNCTIONAL
circ \sim mu age !r str(tree age.tree us(2).tree !INIT 4.6 .00001 .000094),
idv(spl(age,7) !INIT .1) idv(spl(age,7).tree !INIT 2.3),
idv(fac(age) !INIT 13.9)
residual idv(units)
```
## 3.9 Generalised linear (mixed) models

The following is a comparison of the structural and functional specifications for the two examples in Section 16.10 of the ASReml User Guide: Structural Specification. These examples are not presented in full in the ASReml User Guide: Functional Specification.

#### 3.9.1 Binomial analysis of Footrot score

```
Lamb data from ARG thesis page 177-8
Year GRP 5 !V99=V2 !==4 !M1
SEX SIRE !I
Total
FS1 FS2 Scald !+V99 Rot !+V99
pRot !=Rot !/Total
#1 1 1 101 39 33 6 6 1
LAMB.DAT !skip 1
!DF 1904 !YSS 62.54249
#STRUCTURAL AND IMPLICIT FUNCTIONAL
pRot !TOTAL=Total ∼ mu SEX GRP !r SIRE
#EXPLICIT FUNCTIONAL
pRot !TOTAL=Total ∼ mu SEX GRP !r idv(SIRE)
residual idv(units)
```
An analysis of footrot as a binomial variable using the logistic link is performed by the model line (and dropping the !DF qualifier) #STRUCTURAL AND IMPLICIT FUNCTIONAL Rot !BIN !TOTAL=Total mu SEX GRP SEX.GRP !r SIRE .16783 #EXPLICIT FUNCTIONAL Rot !BIN !TOTAL=Total mu SEX GRP SEX.GRP !r idv(SIRE !INIT .16783)

#### 3.9.2 Bivariate analysis of Footrot score

```
Lamb data from ARG thesis page 177-8
Year GRP 5 !V99=V2 !==4 !M 1
SEX SIRE !I
Score1
Score2 Scald !+V99 Rot !+V99
YVar
binnor.asd !skip 1 !ASUV !MAXIT 40
#STRUCTURAL
Score1 YVar !bin ∼ Trait.SEX Trait.GRP !r Trait.SIRE
1 \t2 \t12513
2 0 US !GFPP
1 .01 0.25
Trait.SIRE 2
Trait 0 US 0.015 0.01 1.05
SIRE 0 ID
#FUNCTIONAL
Score1 YVar !bin ∼ Trait.SEX Trait.GRP !r us(Trait).id(SIRE)
residual id(units).us(Trait !INIT 1 -.01 .25 !GFPP)
```
### 3.10 Multivariate animal genetics data - Sheep

```
!RENAME 1 !ARG 1 2 3 4 5 #Does 5 runs one for each trait
Multivariate Sire & Dam model
!DOPATH $1
!IF $1 == 1 !ASSIGN YV wwt #sets up dependent variable to each trait in turn
!IF $1 == 2 !ASSIGN YV ywt
IIF $1 == 3 !ASSIGN YV gfw
IIF $1 == 4 !ASSIGN YV fdm
IIF $1 == 5 !ASSIGN YV fat
tag
sire 92 !I
dam 3561 !I
grp 49
sex
brr 4
litter 4871
```
age wwt !M0 # !M0 identifies missing values ywt !M0 gfw !M0 fdm !M0 fat !M0 coop.fmt #STRUCTURAL !PATH 1 2 3 5 \$YV mu age brr sex age.sex !r sire dam lit age.grp sex.grp !f grp #traits are substituted for \$YV !PATH 4 #leaves out sex.grp for fdm \$YV mu age brr sex age.sex !r idv(sire) idv(dam) idv(lit) idv(age.grp) !f grp #\$fdm is substit #FUNCTIONAL !PATH 1 2 3 5 \$YV mu age brr sex age.sex !r idv(sire) idv(dam) idv(lit) idv(age.grp) idv(sex.grp) !f grp #traits are substituted for\$YV !PATH 4 #leaves out sex.grp for fdm \$YV mu age brr sex age.sex !r idv(sire) idv(dam) idv(lit) idv(age.grp) !f grp #\$fdm is #substituted for \$YV !RENAME 1 !ARG 3 #CHANGE 1 TO 2 OR 3 FOR OTHER PATHS Multivariate Sire & Dam !DOPATH \$1 tag sire 92 !I dam 3561 !I grp 49 sex brr 4 litter 4871 age wwt !M0 # !M0 identifies missing values ywt !M0 gfw !M0 fdm !M0 fat !M0 !PATH 1 // coop.fmt !PATH 2 // coop.fmt !CONTINUE !PATH 3 // coop.fmt !CONTINUE !PATH 0 #USING SUBSET TO SET UP COMBINATIONS OF TRAITS USED IN MODEL !SUBSET TrDam123 Trait 1 2 3 0 0 !SUBSET TrLit1234 Trait 1 2 3 4 0 !SUBSET TrAG1245 Trait 1 2 4 5 !SUBSET TrSG123 Trait 1 2 3 0 0 !SUBSET TrDam12 Trait 1 2 0 0 0 !SUBSET TrDa12 Trait 1 2 0 0 0 #USING !ASSIGN TO MAKE SPECIFICATION CLEARER

#STRUCTURAL #ASSIGN SIRE DAM LITTER AND RESIDUAL INITIAL VALUES FROM UNIVARIATE ANALYSES !ASSIGN SDIAGI 0.608 1.298 0.015 0.197 0.035 #Initial sire variances !ASSIGN DDIAGI 2.2 4.14 0.018 !ASSIGN LDIAGI 3.74 0.97 0.019 0.941 !ASSIGN RUSI !< 9.27 0.0 16.48 0.0 0.0 0.14 0.0 0.0 0.0 3.37 0.0 0.0 0.0 0.0 1.14 !> !ASSIGN VARS !< TrAG1245.age.grp, TrSG123.sex.grp !> #FUNCTIONAL #ASSIGN SIRE DAM LITTER AND RESIDUAL INITIAL VALUES FROM UNIVARIATE ANALYSES !ASSIGN SDIAGI !INIT 0.608 1.298 0.015 0.197 0.035 #Initial sire variances !ASSIGN DDIAGI !INIT 2.2 4.14 0.018 !ASSIGN LDIAGI !INIT 3.74 0.97 0.019 0.941 !ASSIGN RUSI !< !INIT 9.27 0.0 16.48 0.0 0.0 0.14 0.0 0.0 0.0 3.37 0.0 0.0 0.0 0.0 1.14 !> !ASSIGN VARF !< diag(TrAG1245 !INIT 0.0024 0.0019 0.0020 0.00026).age.grp, diag(TrSG123 !INIT 0.93 16.0 0.28).sex.grp !> !PATH 1 #DIAGONAL FOR SIRE DAM AND LITTER UNSTRUCTURED FOR RESIDUAL #STRUCTURAL wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r \$VARS, Trait.sire TrDam123.dam TrLit1234.lit , !f Trait.grp 1 2 5 #1 R STRUCTURE WITH 2 COMPONENTS AND 5 G STRUCTURES 0 0 0 #INDEPENDENT ACROSS ANIMALS Trait 0 US !GP #UNSTRUCTURED TRAIT MATRIX INITIAL VALUES FROM UNIVARIATE ANALYSES \$RUSI TrAG1245.age.grp 2 TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026 age.grp 0 ID TrSG123.sex.grp 2 TrSG123 0 DIAG 0.93 16.0 0.28 sex.grp 0 ID Trait.sire 2 Trait 0 DIAG \$SDIAGI sire 0 ID TrDam123.dam 2 TrDam123 0 DIAG \$DDIAGI dam 0 ID TrLit1234.lit 2 TrLit1234 0 DIAG \$LDIAGI lit 0 ID #FUNCTIONAL wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r \$VARF, diag(Trait \$SDIAGI).sire diag(TrDam123 \$DDIAGI).dam diag(TrLit1234 \$LDIAGI ).lit, !f Trait.grp residual id(units).us(Trait \$RUSI)

```
!PATH 2 #CHANGE DIAGONAL TO XFA1 FOR SIRE DAM AND LITTER
#STRUCTURAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
xfa(Trait,1).sire xfa(TrDam123,1).dam xfa(TrLit1234,1).lit ,
!f Trait.grp mv
1 2 5 #1 R STRUCTURE WITH 2 COMPONENTS AND 5 G STRUCTURES
0 0 0 #INDEPENDENT ACROSS ANIMALS
Trait 0 US *
TrAG1245.age.grp 2
TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
xfa(Trait,1).sire 2
xfa(Trait,1) 0 XFA1 * !GP
sire 0 ID
xfa(TrDam123,1).dam 2
xfa(TrDam123,1) 0 XFA1 * !GP
dam 0 ID
xfa(TrLit1234,1).lit 2
xfa(TrLit1234,1) 0 XFA1 * !GP
lit 0 ID
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
xfa1(Trait).sire xfa1(TrDam123).dam xfa1(TrLit1234).lit ,
!f Trait.grp mv
residual id(units).us(Trait)
!PATH 3 #CHANGE XFA1 TO UNSTRUCTURED FOR SIRE AND LITTER
#STRUCTURAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
Trait.sire xfa(TrDam123,1).dam TrLit1234.lit ,
!f Trait.grp mv
1 2 5 #1 R STRUCTURE WITH 2 COMPONENTS AND 5 G STRUCTURES
0 0 0 #INDEPENDENT ACROSS ANIMALS
Trait 0 US *
TrAG1245.age.grp 2
TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
```

```
Trait.sire 2
Trait 0 US !GP *
sire 0 ID
xfa(TrDam123,1).dam 2
xfa(TrDam123,1) 0 XFA1 *
dam 0 ID
TrLit1234.lit 2
TrLit1234 0 US *
lit 0 ID
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
us(Trait).sire xfa1(TrDam123).dam us(TrLit1234).lit ,
!f Trait.grp mv
residual id(units).us(Trait)
!PATH 3 #WORK OUT FUNCTIONS OF PARAMETERS FOR PATH 3
VPREDICT !DEFINE
X Damv 38:43 # defines 54:59
F phenWYG 1:6 + 23:28 + 54:59 + 44:49 # defines 60:65
F phenD 7:10 + 29:32 + 50:53 # defines 66:69
F phenF 11:15 + 33:37 # defines 70:74
F Direct 23:37 * 4. # defines 75:89
F Maternal 54:59 - 23:28 # defines 90:95
F Resid 60:74 - 75:89 # defines 96:110
H WWTh2 75 60
H YWTh2 77 62
H GFWh2 80 65
H FDMh2 84 69
H FATh2 89 74
R GenCor 23:37
R MatCor 90:95
#STRUCTURAL
VPREDICT !DEFINE
X Damv xfa(TrDam123,1) # defines 54:59
F phenWYG Residual[1:6]+sire[1:6]+TrLit1234.lit[1:6]+Damv
# defines 60:65= 1:6 + 23:28 + 44:49 + 54:59
F phenD Residual[7:10]+Trait.sire[7:10]+ TrLit1234.lit[7:10]
# defines 66:69= 7:10 + 29:32 + 50:53
F phenF Residual[11:15]+Trait.sire[11:15]
# defines 70:74= 11:15 + 33:37
F Direct Trait.sire *4. #defines 75: 89= 23:37 * 4.
F Maternal Damv -Trait[1:6] #defines 90: 95= 54:59 - 23:28
```

```
F residWYG phenWYG - Trait.sire[1:6] #defines 96:101= 60:65 - 23:28F residWYG phenD - Trait.sire[7:10] #defines 102:105= 66:69 - 29:32
F residWYG phenF - Trait.sire[11:15] #defines 106:110= 70:74 - 33:37
#defines 96:110= 60:74 - 23-37
H WWTh2 Direct[1] phenWYG[1] # 75 60
H YWTh2 Direct[3] phenWYG[3] # 77 62
H GFWh2 Direct[6] phenWYG[6] # 80 65
H FDMh2 Direct[10] phenD[4] # 84 69
H FATh2 Direct[15] phenF[5] # 89 74
R GenCor Trait.sire # 23:37
R MatCor Maternal # 90:95
#FUNCTIONAL
VPREDICT !DEFINE
#USING !ASSIGN TO GIVE CONCISE VPREDICT
!ASSIGN lusT lit;us(TrLit1234) # us(TrLit1234).id(lit);us(TrLit1234)
!ASSIGN susT sire;us(Trait) #us(Trait).id(sire);us(Trait)
!ASSIGN uusT id(units).us(Trait);us(Trait)
X Damv xfa1(TrDam123) # defines 54:59
F phen $uusT[1:6]+$susT[1:6]+$lusT[1:6]+xfa1(TrDam123)
# defines [1:6] elements of phen
# defines 60:65= 1:6 + 23:28 + 44:49 + 54:59
F phen $uusT[7:10]+$susT[7:10]+ $lusT[7:10]
# defines [7:10] elements of phen
# defines 66:69= 7:10 + 29:32 + 50:53
F phen $uusT[11:15]+$susT[11:15]
# defines [11:15] elements of phen
# defines 70:74= 11:15 + 33:37
F Direct $susT *4. #defines 75: 89= 23:37 * 4.
F Maternal Damv -$susT[1:6] #defines 90: 95= 54:59 - 23:28
F resid phen - $susT #defines 96:110= 60:74 - 23-37
H WWTh2 Direct[1] phen[1] #defines 111= 75/ 60
H YWTh2 Direct[3] phen[3] #defines 112= 77/ 62
H GFWh2 Direct[6] phen[6] #defines 113= 80/ 65
H FDMh2 Direct[10] phen[10] #defines 114= 84/ 69
H FATh2 Direct[15] phen[15] #defines 115= 89/ 74
R GenCor $susT #defines 116:125 from 23:37
R MatCor Maternal #defines 126:129 from 90:95
!RENAME 1 !ARG 3 #CHANGE 1 TO 2,3,4 OR 5 FOR OTHER PATHS
Multivariate Animal model
!DOPATH $1
tag !P
```
sire 92 !I dam !P

grp 49

```
sex
brr 4
litter 4871
age
wwt !M0 # !M0 identifies missing values
ywt !M0
gfw !M0
fdm !M0
fat !M0
pcoop.fmt # read pedigree from first three fields
!PATH 1 // pcoop.fmt
!PATH 2 // pcoop.fmt !CONTINUE !MAXI 40
!PATH 3 // pcoop.fmt !CONTINUE !MAXI 40
!PATH 4 // pcoop.fmt !CONTINUE !MAXI 40
!PATH 5 // pcoop.fmt !CONTINUE !MAXI 40
!PATH 0 #USING SUBSET TO ALLOW EASY TRAIT ASSOCIATION WITH FACTORS IN MODEL
!SUBSET TrDam12 Trait 1 2 0 0 0
!SUBSET TrLit1234 Trait 1 2 3 4 0
!SUBSET TrAG1245 Trait 1 2 4 5
!SUBSET TrSG123 Trait 1 2 3 0 0
!SUBSET TrDa123 Trait 1 2 3 0 0
#USING !ASSIGN TO MAKE SPECIFICATION CLEARER
#STRUCTURAL
!ASSIGN TDIAGI 2.3759 6.2256 0.60075E-01 0.63086 0.13069 !GP
!ASSIGN DDIAGI 2.1584 2.3048 !GP
!ASSIGN LDIAGI 3.55265 2.55777 0.191238E-01 0.897272 !GP
!ASSIGN RUSI !< !GP
13.390 9.0747 17.798 0.31961 0.87272 0.13452
0.71374 1.4028 0.23141 4.0677 0.72812 2.0831 0.75977E-01 0.25782 1.5337 !>
!ASSIGN VARS TrAG1245.age.grp TrSG123.sex.grp
#FUNCTIONAL
!ASSIGN TDIAGI !INIT 2.3759 6.2256 0.60075E-01 0.63086 0.13069 !GP
!ASSIGN DDIAGI !INIT 2.1584 2.3048 !GP
!ASSIGN LDIAGI !INIT 3.55265 2.55777 0.191238E-01 0.897272 !GP
!ASSIGN RUSI !< !INIT 13.390 9.0747 17.798 0.31961 0.87272 0.13452
0.71374 1.4028 0.23141 4.0677 0.72812 2.0831 0.75977E-01 0.25782 1.5337 !GP !>
!ASSIGN VARF !<
diag(TrAG1245 !INIT 0.0024 0.0019 0.0020 0.00026).age.grp,
diag(TrSG123 !INIT 0.93 16.0 0.28).sex.grp !>
```

```
!PATH 1 #USING DIAG FOR TAG,DAM AND LIT US FOR RESIDUAL
#STRUCTURAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
Trait.tag TrDam12.dam TrLit1234.lit ,
!f Trait.grp
1 2 5 #1 R STRUCTURE WITH 2 COMPONENTS AND 5 G STRUCTURES
0 0 0 #INDEPENDENT ACROSS ANIMALS
Trait 0 US $RUSI #UNSTRUCTURED TRAIT MATRIX INITIAL VALUES FROM UNIVARIATE ANALYSETrAG1245.age.grp
\mathcal{D}TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
Trait.tag 2
Trait 0 DIAG $TDIAGI
tag 0 AINV
TrDam12.dam 2
TrDam12 0 DIAG $DDIAGI
dam 0 ID
TrLit1234.lit 2
TrLit1234 0 DIAG $LDIAGI
lit 0 ID
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
diag(Trait $TDIAGI).nrm(tag) diag(TrDam12 $DDIAGI).dam diag(TrLit1234 $LDIAGI).lit ,
!f Trait.grp
residual id(units).us(Trait $RUSI)
!PATH 2 #USING XFA1 FOR TAG,DAM AND LIT US FOR RESIDUAL
#STRUCTURAL
wwt ywt gfw fdm fat !SIGMAP Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
xfa(Trait,1).tag xfa(TrDam12,1).dam xfa(TrLit1234,1).lit ,
!f Trait.grp
1 2 5
0 0 0
Trait 0 US $RUSI
TrAG1245.age.grp 2
TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
```

```
xfa(Trait,1).tag 2
xfa(Trait,1) 0 KFA1 * !GPtag 0 AINV
xfa(TrDam12,1).dam 2 * !GPxfa(TrDam12,1) 0 XFA1
dam 0 ID
xfa(TrLit1234,1).lit 2 * !GP
xfa(TrLit1234,1) 0 XFA1
lit 0 ID
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
xfa1(Trait).nrm(tag) xfa1(TrDam12).dam xfa1(TrLit1234).lit ,
!f Trait.grp
residual id(units).us(Trait)
!PATH 3
#STRUCTURAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
Trait.tag xfa(TrDam12,1).dam TrLit1234.lit ,
!f Trait.grp
1 2 5
0 0 0
Trait 0 US !GP *
TrAG1245.age.grp 2
TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
Trait.tag 2
Trait 0 US * !GP
tag 0 AINV
xfa(TrDam12,1).dam 2
xfa(TrDam12,1) 0 XFA1 * !GPdam 0 ID
TrLit1234.lit 2
TrLit1234 0 US * !GP
lit 0 ID
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
us(Trait).nrm(tag) xfa1(TrDam12).dam us(TrLit1234).lit ,
!f Trait.grp
residual id(units).us(Trait)
!PATH 4 #FITTING XFA2 FOR TAG
#STRUCTURAL
```

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```

```
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
xfa(Trait,2).tag xfa(TrDam12,1).dam TrLit1234.lit ,
!f Trait.grp
1 2 5
0 0 0
Trait 0 US !GP
TrAG1245.age.grp 2
TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
xfa(Trait,2).tag 2
xfa(Trait,2) 0 XFA2 *!GP
tag 0 AINV
xfa(TrDam12,1).dam 2
xfa(TrDam12,1) 0 KFA1 * !GPdam 0 ID
TrLit1234.lit 2
TrLit1234 0 US * !GP
lit 0 ID
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
xfa2(Trait).nrm(tag) xfa1(TrDam12).dam us(TrLit1234).lit ,
!f Trait.grp
residual id(units).us(Trait)
!PATH 5 #FITTING XFA3 FOR TAG
#STRUCTURAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARS,
xfa(Trait,3).tag xfa(TrDam12,1).dam TrLit1234.lit ,
!f Trait.grp
1 2 5
0 0 0
Trait 0 US !GP
TrAG1245.age.grp 2
TrAG1245 0 DIAG 0.0024 0.0019 0.0020 0.00026
age.grp 0 ID
TrSG123.sex.grp 2
TrSG123 0 DIAG 0.93 16.0 0.28
sex.grp 0 ID
xfa(Trait,3).tag 2
xfa(Trait,3) 0 XFA3 * !GP
tag 0 AINV
xfa(TrDam12,1).dam 2
xfa(TrDam12,1) 0 XFA1 * !GPdam 0 ID
```

```
TrLit1234.lit 2
TrLit1234 0 US * !GP
lit 0 ID
!PATH 5
#FUNCTIONAL
wwt ywt gfw fdm fat Trait Trait.age Trait.brr Trait.sex Trait.age.sex !r $VARF,
xfa3(Trait).nrm(tag) xfa1(TrDam12).dam us(TrLit1234).lit ,
!f Trait.grp
residual id(units).us(Trait)
```
# Bibliography

Wolfinger, R. D. (1996). Heterogeneous variance-covariance structures for repeated measures, Journal of Agricultural, Biological, and Environmental Statistics 1: 362–389.