

BreedR Overview

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Intro

What is breedR

- R-package implementing **statistical models** specifically suited for forest genetic resources analysts.
- Ultimately [Mixed Models](#), but not necessarily easy to implement and use
- **breedR** acts as an **interface** which provides the means to:
 1. **Combine** any number of these models as **components** of a larger model
 2. Compute automatically **incidence** and **covariance matrices** from a few input parameters
 3. **Fit** the model
 4. Plot data and results, and perform **model diagnostics**

Installation

- Project web page <http://famuvie.github.io/breedR/>
 - download .zip or .tar.gz source files
 - `install.packages('famuvie-breedR-*', type = 'source', repos = NULL)`
- GitHub dev-site <https://github.com/famuvie/breedR>
 - `if(!require(devtools)) install.packages('devtools')`
 - `devtools::install_github('famuvie/breedR')`
- CRAN not there yet... but soon
 - `install.packages('breedR')`

Where to find help

- Package's help: `help(package = breedR)`
 - Help pages
 - Code demos `demo(topic, package = 'breedR')` (omit topic for a list)
 - Vignettes (none yet)
- Wiki pages
 - Guides, tutorials, FAQ
- Mailing list <http://groups.google.com/group/breedr>
 - Questions and debates about usage and interface
- Issues page
 - Bug reports
 - Feature requests

License



- **breedR** is FOSS. Licensed [GPL-3](#)
 - `RShowDoc('LICENSE', package = 'breedR')`
- You can **use** and **distribute breedR** for any purpose
- You can **modify** it to suit your needs
 - we encourage to!
 - please consider contributing your improvements
 - you can **distribute** your modified version under the GPL
- However, **breedR** makes (intensive) use of the [BLUPF90](#) suite of Fortran programs, which **are not free**

Roadmap | Future developments

- Bayesian inference
- Multi-trait support
- Genotype×Environment interaction
- Support for longitudinal data

Functionality

Inference

Frequentist

- Currently, only **frequentist inference** is supported via REML estimation of variance components.
- The function `remlf90()`, provides an interface to both `REMLF90` and `AIREMLF90` functions in the [BLUPF90](#) suite of Fortran programs.
- Type `?remlf90` for details on the syntax

Bayesian

- It's on the roadmap for the next year
- Will use a gibbs sampler from [BLUPF90](#), and possibly also [INLA](#)
- The **interface** will change a bit, separating the model specification from the fit

Linear Mixed Models with unstructured random effects

Example dataset

self	dad	mum	gen	gg	bl	phe_X	x	y	fam
69	0	64	1	14	13	15.756	0	0	64
70	0	41	1	4	13	11.141	3	0	41
71	0	56	1	14	13	19.258	6	0	56
72	0	55	1	14	13	4.775	9	0	55
73	0	22	1	8	13	19.099	12	0	22
74	0	50	1	14	13	19.258	15	0	50

```
## 'data.frame': 1021 obs. of 10 variables:
## $ self : int 69 70 71 72 73 74 75 76 77 78 ...
## $ dad : int 0 0 0 0 0 0 0 0 0 4 ...
## $ mum : int 64 41 56 55 22 50 67 59 49 8 ...
## $ gen : Factor w/ 1 level "1": 1 1 1 1 1 1 1 1 1 1 ...
## $ gg : Factor w/ 14 levels "1","2","3","4",...: 14 4 14 14 8 14 14 14 14 11 ...
```

```
## $ bl : Factor w/ 15 levels "1","2","3","4",...: 13 13 13 13 13 13 13 13 9 9 ...
## $ phe_X: num 15.76 11.14 19.26 4.78 19.1 ...
## $ x : int 0 3 6 9 12 15 18 21 24 27 ...
## $ y : int 0 0 0 0 0 0 0 0 0 0 ...
## $ fam : Factor w/ 63 levels "6","7","8","9",...: 59 36 51 50 17 45 62 54 44 3 ...
```

A simple Provenance Test

Specify the *genetic group* `gg` as an **unstructured random effect** using the standard formulas in R

$$\begin{aligned} \text{phe}_X &= \mu + Z_{gg} + \varepsilon \\ gg &\sim N(0, \sigma_{gg}^2) \\ \varepsilon &\sim N(0, \sigma_{\varepsilon}^2) \end{aligned}$$

```
res <- remlf90(fixed = phe_X ~ 1,
              random = ~ gg,
              data = globulus)
```

```
## No specification of initial variances.
## Using default value of 1 for all variance components.
## See ?breedR.getOption.
```

Initial variances specification

To avoid the notification, initial values for *all* the variance components must be made explicit using the argument `var.ini`:

```
res <- remlf90(fixed = phe_X ~ 1,
              random = ~ gg,
              var.ini = list(gg = 2, resid = 10),
              data = globulus)
```

Although in most cases the results will not change at all, we encourage to give explicit initial values for variance components. Specially when some estimate can be [artifact](#). This is also useful for checking sensitivity to initial values.

Exploring the results

```
summary(res)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
## Data: globulus
## AIC BIC logLik
## 5864 5874 -2930
##
## Parameters of special components:
##
##
```

```
## Variance components:
##           Estimated variances   S.E.
## gg                2.857 1.3584
## Residual          17.695 0.7888
##
## Fixed effects:
##           value   s.e.
## Intercept 14.799 0.4911
```

- Note that AI-REML has been used by default.
- You can also specify `method = 'em'`.
- Learn about the [difference](#).

Further *extractor* functions

```
fixef(res)
```

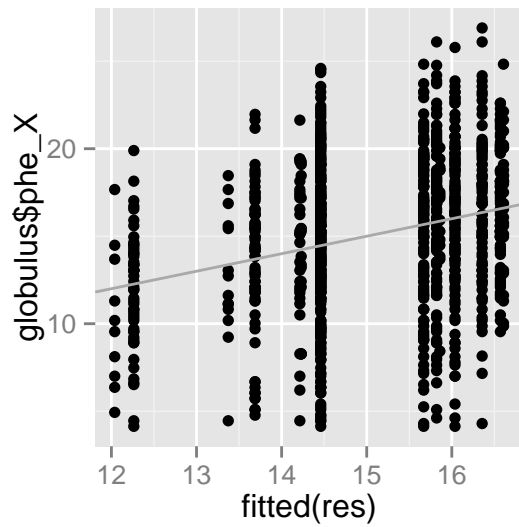
```
## $Intercept
##      value      s.e.
## 1 14.79913 0.4910935
```

```
ranef(res)
```

```
## $gg
##      value      s.e.
## 1 -1.1113032 0.6582248
## 2 -0.5850024 0.8241564
## 3  1.2381745 0.6017960
## 4 -2.5360696 0.7047334
## 5  1.0223495 0.6298412
## 6 -2.7605972 1.0884708
## 7 -0.5691185 0.9776415
## 8  0.8700427 0.5933967
## 9  1.5572487 0.6381501
## 10 -1.4262293 0.9961142
## 11  1.7715259 0.6527005
## 12  1.8079965 0.8241564
## 13  1.0604399 0.9776415
## 14 -0.3394576 0.5380187
```

Further *extractor* functions

```
qplot(
  fitted(res),
  globulus$phe_X) +
  geom_abline(int = 0,
    sl = 1,
    col = 'darkgrey')
```



```
str(resid(res))
```

```
## Named num [1:1021] 1.3 -1.12 4.8 -9.68 3.43 ...
## - attr(*, "names")= chr [1:1021] "1" "2" "3" "4" ...
```

```
extractAIC(res)
```

```
## [1] 5863.716
```

```
logLik(res)
```

```
## 'log Lik.' -2929.858 (df=2)
```

Hierarchical and Factorial models

- In globulus, the **family** (mum) is *nested* within the **provenance** (gg)
- This is a matter of codification:

Nested factors

gg	mum
A	1
A	2
B	3
B	4

Crossed factors

gg	mum
A	1
A	2

gg	mum
B	1
B	2

- Otherwise, in both cases we specify the same thing

```
random = ~ gg + factor(mum) # note that mum is numeric
```

- Furthermore, this approach can handle unbalanced and mixed designs

Interactions

- Standard R notation:

```
random = ~ gg * factor(mum)
```

- Not available yet (feature request?)
- Workaround: build the interaction variable manually
- Example: gg and bl are crossed factors

```
dat <- transform(globulus,
                 interaction = factor(gg:bl))
random = ~ gg + bl + interaction
```

Exercise | Hierarchical and Factorial models

1. Use `remlf90()` and the globulus dataset to fit
 - a hierarchical model using mum **within** gg
 - a factorial model using gg and bl
2. Explore the results with `summary()`
 - is the family (mum) effect **relevant**?
 - is there any evidence of interaction between gg and bl?

Hierarchical and Factorial models #1 | Fitting models

```
res.h <- remlf90(fixed = phe_X ~ 1,
                random = ~ factor(mum) + gg,
                data = globulus)
```

```
# Interaction variable
globulus.f <- transform(globulus,
                      gg_bl = factor(gg:bl))

res.f <- remlf90(fixed = phe_X ~ 1,
                random = ~ gg + bl + gg_bl,
                data = globulus.f)
```

Hierarchical and Factorial models #2 | Hierarchical model

- The family effect is not very **important**, in terms of explained variance
- However, the model is a bit better with it (AIC, logLik)

```
summary(res)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
##   Data: globulus
##   AIC  BIC logLik
##  5864 5874  -2930
##
## Parameters of special components:
##
##
## Variance components:
##           Estimated variances   S.E.
## gg                        2.857 1.3584
## Residual                  17.695 0.7888
##
## Fixed effects:
##           value   s.e.
## Intercept 14.799 0.4911
```

```
summary(res.h)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
##   Data: globulus
##   AIC  BIC logLik
##  5857 5872  -2926
##
## Parameters of special components:
##
##
## Variance components:
##           Estimated variances   S.E.
## factor(mum)           0.8955 0.4177
## gg                    2.0540 1.1706
## Residual              17.0770 0.7819
##
## Fixed effects:
##           value   s.e.
## Intercept 14.973 0.4702
```

Hierarchical and Factorial models #3 | Factorial model

- Looks like the interaction between **block** and **provenance** is negligible
- (apart from the fact that it makes no sense at all, and should not have been even considered in the first place)
- compare with the model without interaction

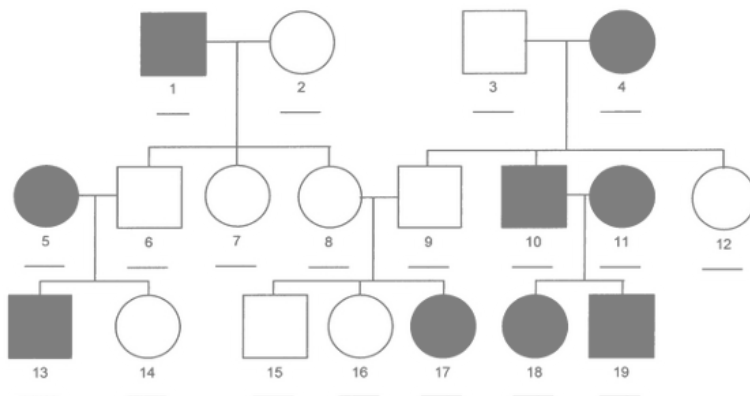

```
summary(res.f)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
##   Data: globulus.f
##   AIC  BIC logLik
## 5752 5772 -2872
##
## Parameters of special components:
##
##
## Variance components:
##           Estimated variances   S.E.
## gg                3.10970 1.4329
## bl                2.57280 1.0606
## gg_bl             0.02912 0.2713
## Residual          15.19800 0.7159
##
## Fixed effects:
##           value  s.e.
## Intercept 14.764 0.653
```

```
## result without interaction
res.f0 <- remlf90(fixed = phe_X ~ 1,
                  random = ~ gg + bl,
                  data = globulus)
paste('AIC:', round(extractAIC(res.f0)),
      'logLik:', round(logLik(res.f0)))
```

```
## [1] "AIC: 5750 logLik: -2872"
```

Additive Genetic Effect



What is an additive genetic effect

- Random effect at **individual level**

- Based on a **pedigree**
- BLUP of **Breeding Values** from own and relatives' phenotypes
- Represents the **additive component** of the genetic value
- More general:
 - family effect is a particular case
 - accounts for more than one generation
 - mixed relationships
- More flexible: allows to select individuals within families

Specifying a *pedigree*

- A 3-column `data.frame` or `matrix` with the codes for each individual and its parents
- A **family** effect is easily translated into a pedigree:
 - use the **family code** as the identification of a fictitious **mother**
 - use 0 or NA as codes for the **unknown fathers**

self	dad	mum
69	0	64
70	0	41
71	0	56
72	0	55
73	0	22
74	0	50

Fitting an *animal model*

```
res.animal <- remlf90(fixed = phe_X ~ 1,
                     random = ~ gg,
                     genetic = list(model = 'add_animal',
                                    pedigree = globulus[, 1:3],
                                    id = 'self'),
                     data = globulus)
```

Animal model: results

```
summary(res.animal)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
##   Data: globulus
##   AIC  BIC logLik
```

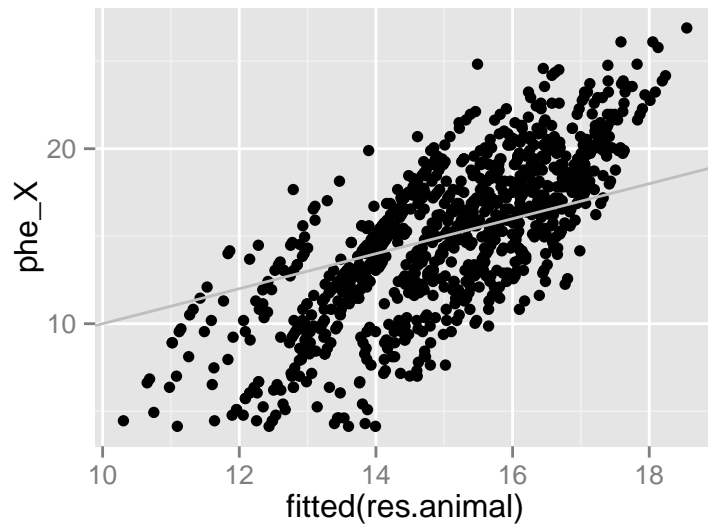
```
## 5857 5872 -2926
##
## Parameters of special components:
##
##
## Variance components:
##           Estimated variances  S.E.
## gg                2.356 1.249
## genetic            3.632 1.649
## Residual           14.271 1.561
##
##           Estimate    S.E.
## Heritability    0.1795 0.08253
##
## Fixed effects:
##           value s.e.
## Intercept 14.797 0.47
```

- **gg** explains almost the same amount of phenotypic variability
- The (additive) **genetic** effect explains **part** of the formerly residual variance
- The heritability is computed automatically as $h^2 = \frac{\sigma_a^2}{\sigma_a^2 + \sigma^2}$

Extracting Predicted Breeding Values

```
## Predicted Breeding Values
# for the full pedigree first, and for the observed individuals
# by matrix multiplication with the incidence matrix
PBV.full <- ranef(res.animal)$genetic
PBV <- model.matrix(res.animal)$genetic %*% PBV.full

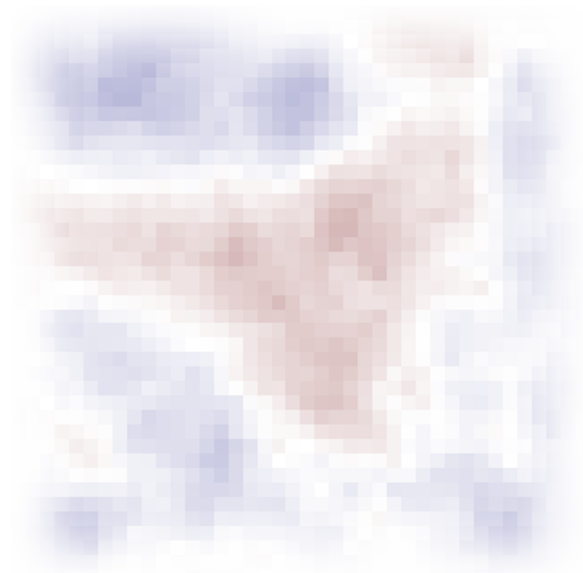
# Predicted genetic values vs.
# phenotype.
# Note: fitted = mu + PBV
qplot(fitted(res.animal), phe_X,
      data = globulus) +
  geom_abline(int = 0,
              slope = 1,
              col = 'gray')
```



Handling pedigrees

- The pedigree needs to meet certain conditions
- If it does not, **breedR** automatically completes, recodes and sorts
- If recoding is necessary, **breedR** issues a warning because you need to be careful when retrieving results
- See this [guide](#) for more details

Spatial autocorrelation



What is spatial autocorrelation

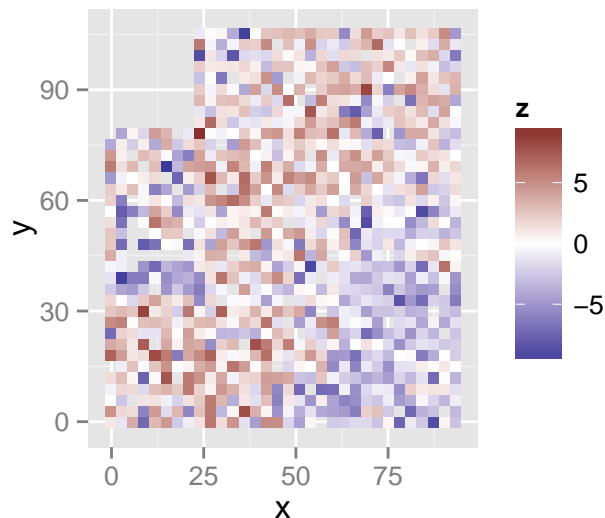
- The **residuals** of any LMM must be **noise**

- However, most times there are **environmental factors** that affect the response
- This causes that observations that are close to each other **tend** to be more similar than observations that are far away
- This is called **spatial autocorrelation**
- It may affect both the estimations and their accuracy
- This is why experiments are randomized into spatial **blocks**

Diagnosing spatial autocorrelation | residuals spatial plot

- You can `plot()` the spatial arrangement of various model components (e.g. residuals)
- Look like **independent** gaussian observations (i.e. noise)?
- Do you see any **signal** in the background?

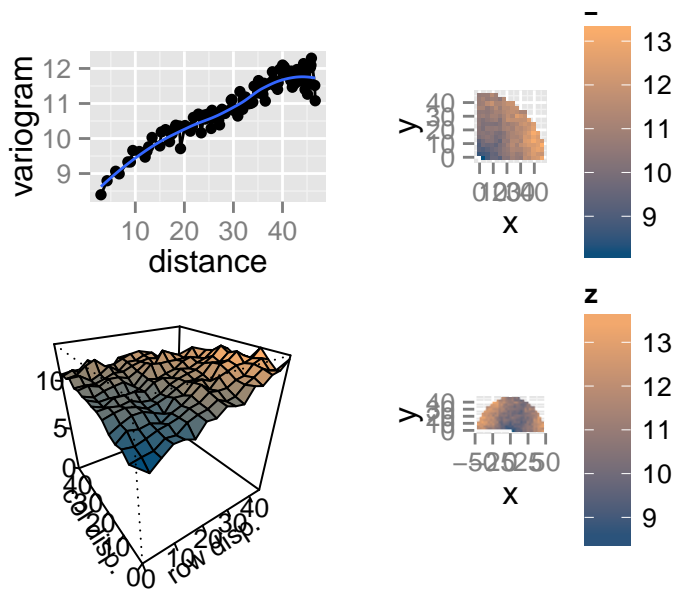
```
## Since coordinates have not
## been passed before they
## must be provided explicitly.
coordinates(res.animal) <-
  globulus[, c('x', 'y')]
plot(res.animal, 'resid')
```



Diagnosing spatial autocorrelation | variograms of residuals

- Plot the **variogram of residuals** with `variogram()`

```
variogram(res.animal)
```

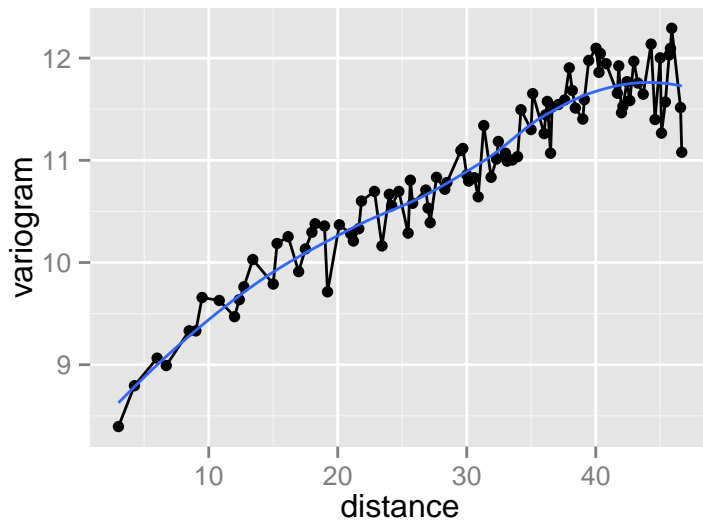


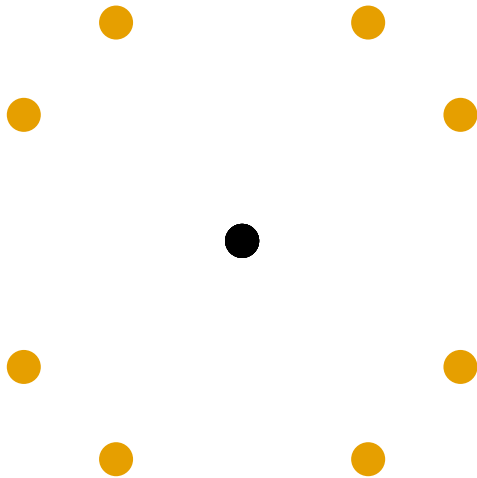
Interpreting the variograms

- Isotropic variogram:

$$\gamma(h) = \frac{1}{2} V[Z(\mathbf{u}) - Z(\mathbf{v})], \quad \text{dist}(\mathbf{u}, \mathbf{v}) = h$$

The **empirical** isotropic variogram is built by aggregating **all the pairs** of points separated by h , **no matter the direction**.



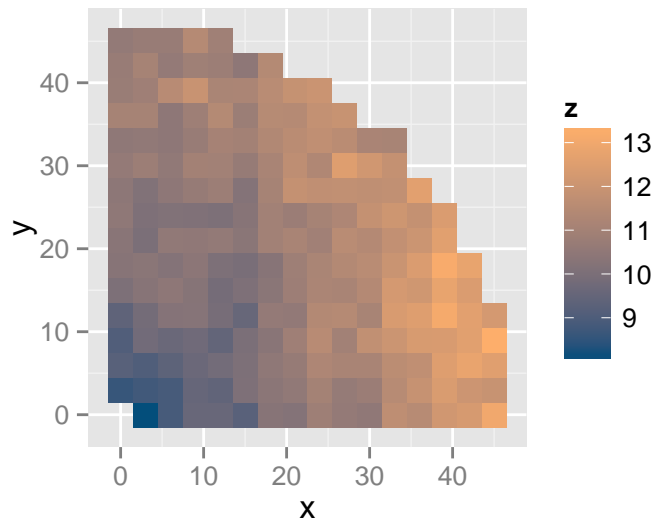


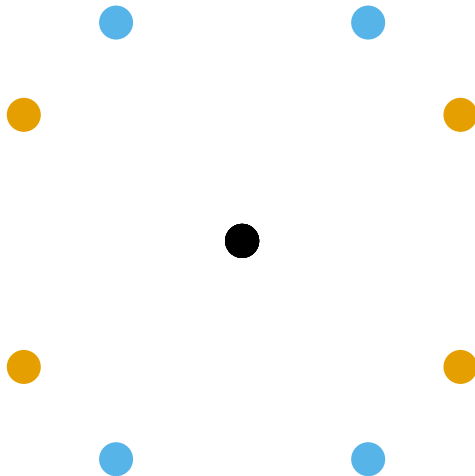
Interpreting the variograms

- Row/Column variogram:

$$\gamma(x, y) = \frac{1}{2} V[Z(\mathbf{u}) - Z(\mathbf{v})], \quad \text{dist}(\mathbf{u}, \mathbf{v}) = (x, y)$$

The **empirical** row/col variogram is built by aggregating **all the pairs** of points separated by exactly x rows and y columns.



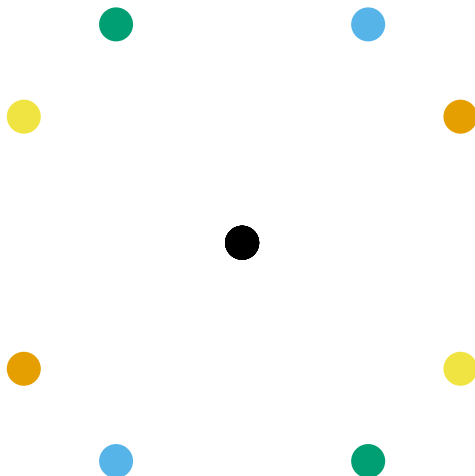
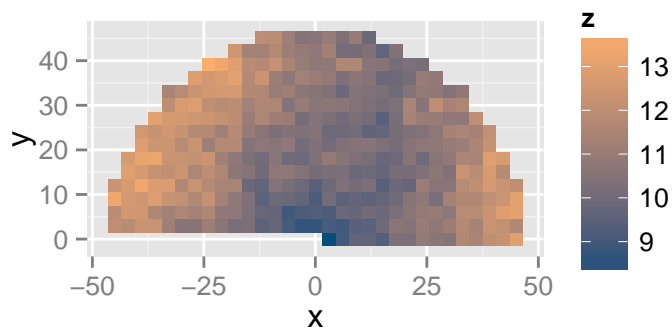


Interpreting the variograms

- Anisotropic variogram:

$$\gamma(\mathbf{x}) = \frac{1}{2} V[Z(\mathbf{u}) - Z(\mathbf{v})], \quad \mathbf{u} = \mathbf{v} \pm \mathbf{x}$$

The **empirical** anisotropic variogram is built by aggregating **all the pairs of points in the same direction** separated by $|\mathbf{x}|$.



Accounting for spatial autocorrelation

- Include an explicit **spatial effect** in the model
- I.e., a **random effect** with a specific covariance structure that reflects the spatial relationship between individuals
- The **block** effect, is a very particular case:
 - It is designed from the beginning, possibly using prior knowledge
 - Introduces **independent** effects between blocks
 - Most neighbours are within the same block (i.e. share the same effect)

The blocks model

```
# The genetic component (DRY)
gen.globulus <- list(model = 'add_animal',
                    pedigree = globulus[, 1:3],
                    id = 'self')

res.blk <- remlf90(fixed = phe_X ~ 1,
                 random = ~ gg,
                 genetic = gen.globulus,
                 spatial = list(model = 'blocks',
                              coord = globulus[, c('x', 'y')],
                              id = 'bl'),
                 data = globulus)
```

- The blocks spatial model is **equivalent** to `random = ~ bl`, but:
 - specifying `coord` is convenient for plotting (remember?)
 - `blocks` behaves as expected, even if `bl` is not a **factor**

Animal-spatial model: results

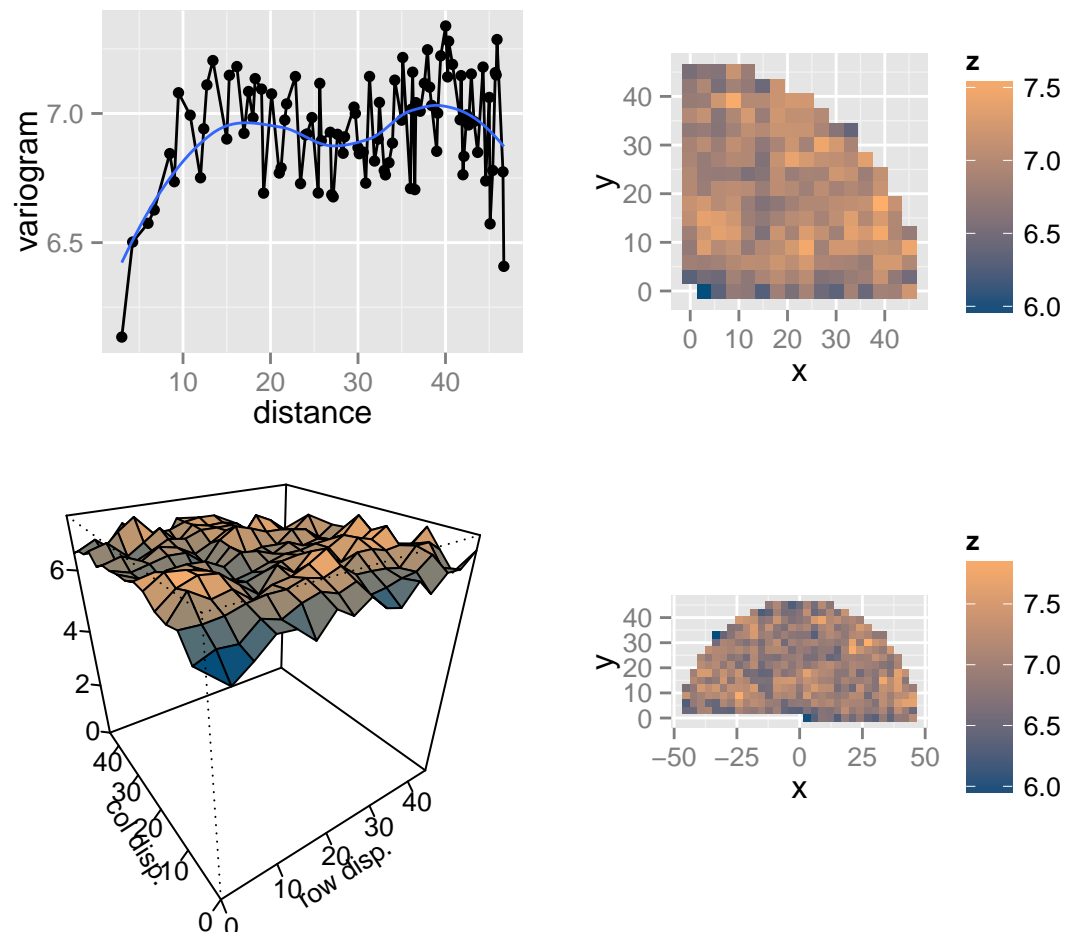
```
summary(res.blk)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
##   Data: globulus
##   AIC  BIC logLik
## 5734 5753 -2863
##
## Parameters of special components:
## spatial: n.blocks: 15
##
## Variance components:
##           Estimated variances  S.E.
## gg                2.385 1.274
## genetic            5.275 1.836
## spatial            2.650 1.081
```

```
## Residual          10.279 1.601
##
##           Estimate   S.E.
## Heritability  0.2556 0.08989
##
## Fixed effects:
##           value   s.e.
## Intercept 14.762 0.6342
```

- Now the additive-genetic variance increased! (3.6 before)

Variogram of residuals



- There seems to remain some intra-block spatial autocorrelation

B-Splines model

- A continuous and smooth spatial surface built from a linear combination of **basis** functions
- The coefficients are modelled as a random effect

```
## Use the `em` method! `ai` does not like splines
res.spl <- remlf90(fixed = phe_X ~ 1,
                  random = ~ gg,
                  genetic = gen.globulus,
                  spatial = list(model = 'splines',
                                coord = globulus[, c('x','y')]),
                  data = globulus, method = 'em')
```

Autoregressive model

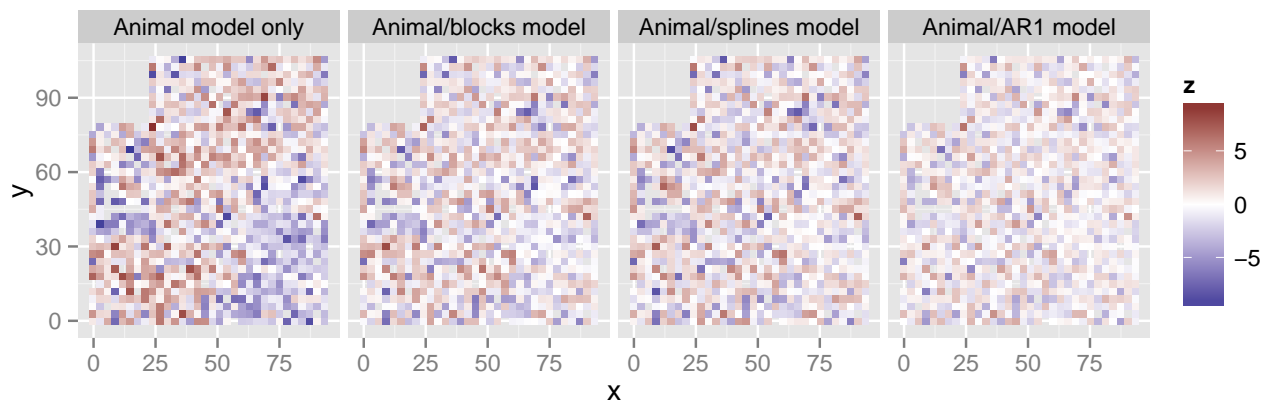
- A separable kronecker product of First order Autoregressive processes on the rows and the columns

```
res.ar1 <- remlf90(fixed = phe_X ~ 1,
                  random = ~ gg,
                  genetic = gen.globulus,
                  spatial = list(model = 'AR',
                                coord = globulus[, c('x','y')]),
                  data = globulus)
```

Change in model residuals

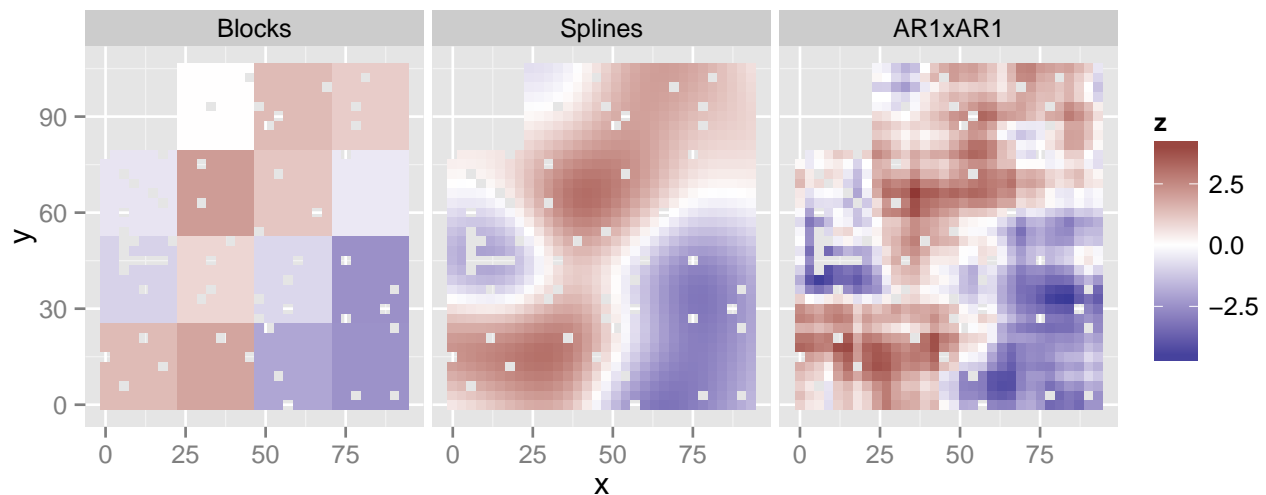
- We preserve the scale by using `compare.plots()`

```
compare.plots(
  list(`Animal model only` = plot(res.animal, 'residuals'),
       `Animal/blocks model` = plot(res.blk, 'residuals'),
       `Animal/splines model` = plot(res.spl, 'residuals'),
       `Animal/AR1 model` = plot(res.ar1, 'residuals')))
```



Comparison of spatial components

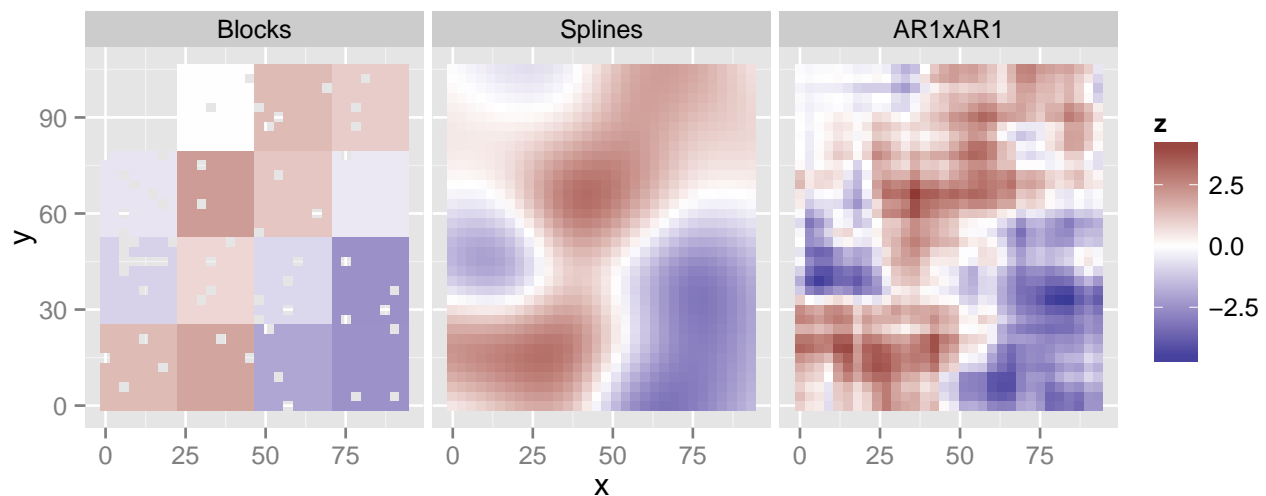
```
compare.plots(list(Blocks = plot(res.blk, type = 'spatial'),
                  Splines = plot(res.spl, type = 'spatial'),
                  AR1xAR1 = plot(res.ar1, type = 'spatial')))
```



Prediction of the spatial effect in unobserved locations

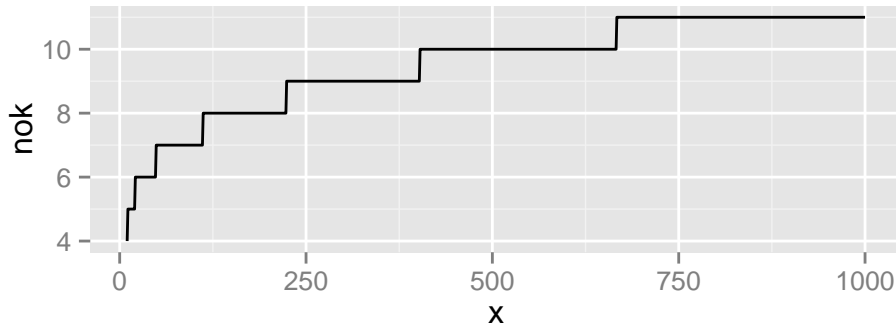
- The type `fullspatial` fills the holes (when possible)
- See `?plot.remlf90`

```
compare.plots(list(Blocks = plot(res.blk, type = 'fullspatial'),
                   Splines = plot(res.spl, type = 'fullspatial'),
                   AR1xAR1 = plot(res.ar1, type = 'fullspatial')))
```



Spatial parameters | Number of knots of a splines model

- The smoothness of the spatial surface can be controlled modifying the number of base functions
- This is, directly determined by the **number of knots** (`nok`) in each dimension
- `n.knots` can be **used as an additional argument** in the spatial effect as a numeric vector of size 2.
- Otherwise, is determined by the function given in `breedR.getOption('splines.nok')`



Spatial parameters | Autoregressive parameters of a AR model

- Analogously, the *patchiness* of the AR effects can be controlled by the autoregressive parameter for each dimension
- **rho** can be **given as an additional argument** in the **spatial** effect as a numeric vector of size 2
- By default, **breedR** runs all the combinations in the grid produced by the values from `breedR.getOption('ar.eval')` and returns the one with largest likelihood
- It returns also the full table of combinations and likelihoods in `res$rho`

Exercise | Tuning spatial parameters

- Tuning parameters:
 - model splines: `n.knots`
 - model AR: `rho`
1. Increase the number of knots in the `splines` model and see if it improves the fit
 2. Visualize the log-likelihood of the fitted AR models
 3. Refine the grid around the most likely values, and refit using `rho = rho.grid`, where

```
rho.grid <- expand.grid(rho_r = seq(.7, .95, length = 4),
                      rho_c = seq(.7, .95, length = 4))
```

- What are now the most likely parameters?

Spatial #1 | B-splines model with increased nok

- `nok` were (6, 6) by default (see `summary()`)

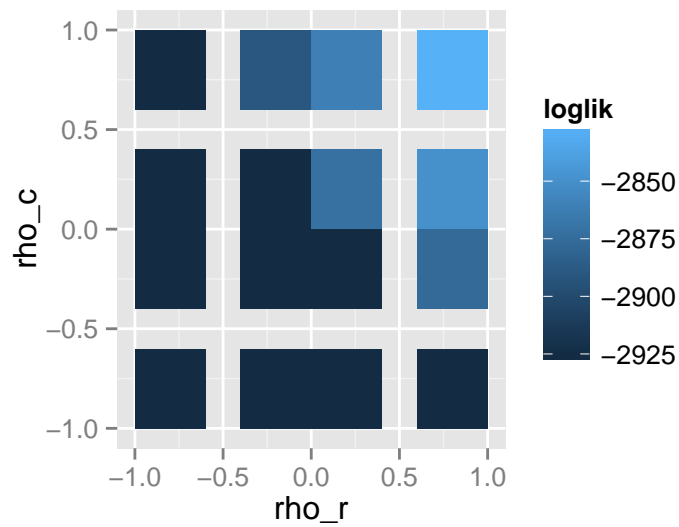
```
res.spl99 <- remlf90(fixed = phe_X ~ 1, random = ~ gg,
                    genetic = gen.globulus,
                    spatial = list(model = 'splines',
                                   coord = globulus[, c('x','y')],
                                   n.knots = c(9, 9)),
                    data = globulus, method = 'em')
```

```
## Linear Mixed Model with pedigree and spatial effects fit by REMLF90 ver. 1.79
##   Data: globulus
##   AIC      BIC logLik
## 5685 unknown -2838
##
## Parameters of special components:
## spatial: n.knots: 12 12
##
## Variance components:
##           Estimated variances
## gg                2.568
## genetic            4.500
## spatial            4.200
## Residual           10.070
##
## Fixed effects:
##           value    s.e.
## Intercept 14.479 0.9163

## Linear Mixed Model with pedigree and spatial effects fit by REMLF90 ver. 1.79
##   Data: globulus
##   AIC      BIC logLik
## 5681 unknown -2836
##
## Parameters of special components:
## spatial: n.knots: 15 15
##
## Variance components:
##           Estimated variances
## gg                2.510
## genetic            4.651
## spatial            3.490
## Residual           9.552
##
## Fixed effects:
##           value    s.e.
## Intercept 14.611 0.6947
```

Spatial #2 | Visualize log-likelihoods

```
qplot(rho_r, rho_c,
      fill = loglik,
      geom = 'tile',
      data = res.ar1$rho)
```



rho_r	rho_c	loglik
-0.8	-0.8	-2925.646
-0.2	-0.8	-2925.646
0.2	-0.8	-2925.646
0.8	-0.8	-2925.636
-0.8	-0.2	-2925.647
-0.2	-0.2	-2925.645
0.2	-0.2	-2925.023
0.8	-0.2	-2876.893
-0.8	0.2	-2925.646
-0.2	0.2	-2925.645
0.2	0.2	-2871.691
0.8	0.2	-2849.814
-0.8	0.8	-2925.645
-0.2	0.8	-2890.606
0.2	0.8	-2860.981
0.8	0.8	-2828.017

Spatial #3 | Refine grid

```
res.ar.grid <- remlf90(fixed = phe_X ~ gg,
                      genetic = list(model = 'add_animal',
                                     pedigree = globulus[,1:3],
                                     id = 'self'),
                      spatial = list(model = 'AR',
                                     coord = globulus[, c('x','y')],
                                     rho = rho.grid),
                      data = globulus)
summary(res.ar.grid)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
## Data: globulus
## AIC BIC logLik
```

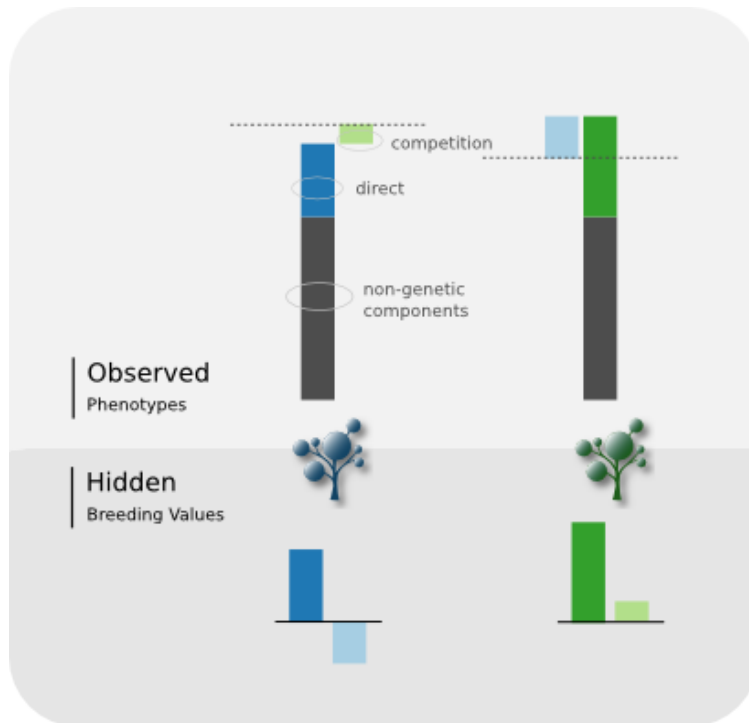
```

## 5603 5617 -2798
##
## Parameters of special components:
## spatial: rho: 0.8666667 0.7833333
##
## Variance components:
##           Estimated variances  S.E.
## genetic                5.090 1.715
## spatial                4.984 1.053
## Residual               7.583 1.499
##
##           Estimate    S.E.
## Heritability  0.2878 0.09383
##
## Fixed effects:
##           value    s.e.
## gg.1  13.351 0.7195
## gg.2  14.331 0.9112
## gg.3  15.945 0.7698
## gg.4  11.585 0.9394
## gg.5  15.913 0.8200
## gg.6   9.593 1.6964
## gg.7  13.761 1.5681
## gg.8  15.521 0.7486
## gg.9  16.302 0.8260
## gg.10 12.684 1.1531
## gg.11 16.459 0.9849
## gg.12 16.801 1.1412
## gg.13 15.783 1.5665
## gg.14 14.211 0.6486

```


Competition

Theoretical model



- Each individual have **two** (unknown) Breeding Values (BV)
- The **direct** BV affects its **own** phenotype, while the **competition** BV affects its **neighbours'** (as the King moves)
- The effect of the neighbouring **competition** BVs is given by their sum **weighted by** $1/d^\alpha$, where α is a tuning parameter called **decay**
- Each set of BVs is modelled as a zero-mean **random effect** with structure matrix given by the **pedigree** and independent **variances** σ_a^2 and σ_c^2
- Both random effects are modelled jointly with **correlation** ρ

Permanent Environmental Effect (pec)

- **Optional** effect with **environmental** (rather than genetic) basis
- Modelled as an individual **independent** random effect that affects **neighbouring** trees in the same (weighted) way

Simulation of data

breedR implements a convenient dataset **simulator** which keeps a similar syntax.

- See ?simulation for details on the syntax

```
# Simulation parameters
grid.size <- c(x=20, y=25) # cols/rows
coord <- expand.grid(sapply(grid.size,
                             seq))

Nobs <- prod(grid.size)
Nparents <- c(mum = 20, dad = 20)
sigma2_a <- 2 # direct add-gen var
sigma2_c <- 1 # compet add-gen var
rho <- -.7 # gen corr dire-comp
sigma2_s <- 1 # spatial variance
sigma2_p <- .5 # pec variance
sigma2 <- .5 # residual variance

S <- matrix(c(sigma2_a,
              rho*sqrt(sigma2_a*sigma2_c),
              rho*sqrt(sigma2_a*sigma2_c),
              sigma2_c),
            2, 2)

set.seed(12345)
simdat <-
  breedR.sample.phenotype(
    fixed = c(beta = 10),
    genetic = list(model = 'competition',
                  Nparents = Nparents,
                  sigma2_a = S,
                  check.factorial=FALSE,
                  pec = sigma2_p),
    spatial = list(model = 'AR',
                  grid.size = grid.size,
                  rho = c(.3, .8),
                  sigma2_s = sigma2_s),
    residual.variance = sigma2
  )

## Remove founders
dat <- subset(simdat,
              !(is.na(simdat$sire)
                & is.na(simdat$dam)))
```

Fitting a competition model

```
system.time(
  res.comp <- remlf90(fixed = phenotype ~ 1,
                    genetic = list(model = 'competition',
                                  pedigree = dat[, 1:3],
                                  id = 'self',
                                  coord = dat[, c('x', 'y')],
                                  competition_decay = 1,
                                  pec = list(present = TRUE)),
```

```

    spatial = list(model = 'AR',
                    coord = dat[, c('x', 'y')],
                    rho    = c(.3, .8)),

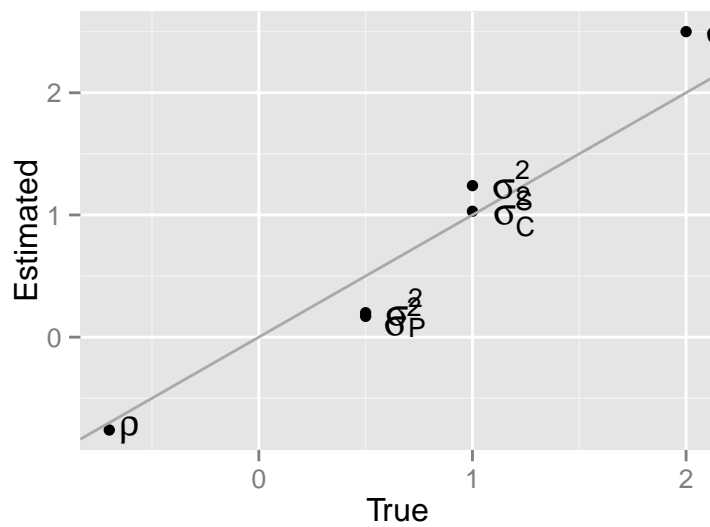
    data = dat,
    method = 'em') # AI diverges
)

```

```
##      user  system elapsed
## 104.708   0.268 105.014
```

True vs. estimated parameters

	True	Estimated
direct	2.0	2.50
compet.	1.0	1.03
correl.	-0.7	-0.76
spatial	1.0	1.24
pec	0.5	0.20
residual	0.5	0.17



Exercise | Competition models

- Plot the true vs predicted:
 - direct and competition Breeding Values
 - spatial effects
 - pec effects
- Plot the residuals and their variogram
 - Do you think the residuals are independent?
 - How would you improve the analysis?

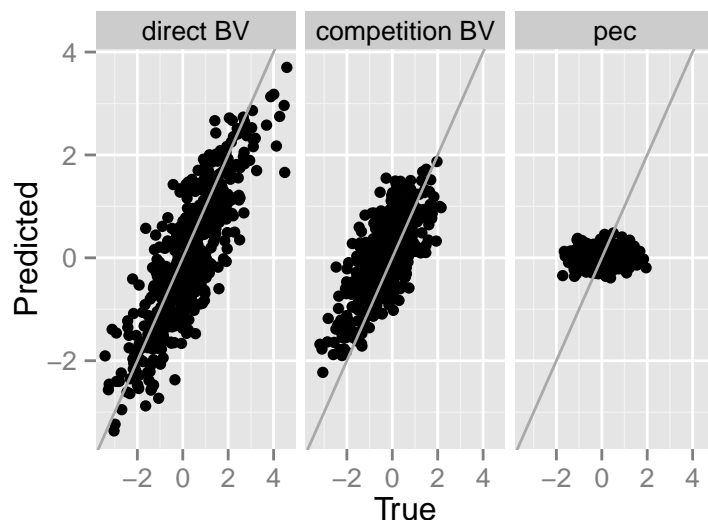
Competition #1 | True vs. predicted components

```
## compute the predicted effects for the observations
## by matrix multiplication of the incidence matrix and the BLUPs
pred <- list()
Zd <- model.matrix(res.comp)$'genetic_direct'
pred$direct <- Zd %*% ranef(res.comp)$'genetic_direct'

## Watch out! for the competition effects you need to use the incidence
## matrix of the direct genetic effect, to get their own value.
## Otherwise, you get the predicted effect of the neighbours on each individual.
pred$comp <- Zd %*% ranef(res.comp)$'genetic_competition'
pred$pec <- as.vector(model.matrix(res.comp)$pec %*% ranef(res.comp)$pec)

comp.pred <-
  rbind(
    data.frame(
      Component = 'direct BV',
      True = dat$BV1,
      Predicted = pred$direct),
    data.frame(
      Component = 'competition BV',
      True = dat$BV2,
      Predicted = pred$comp),
    data.frame(
      Component = 'pec',
      True = dat$pec,
      Predicted = pred$pec))

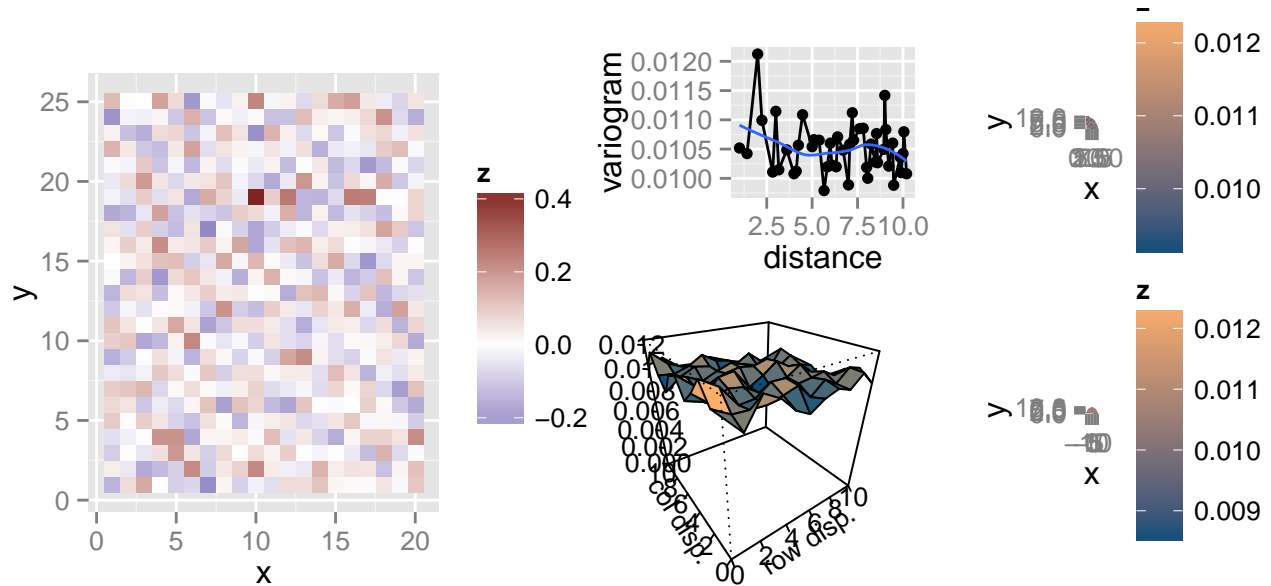
ggplot(comp.pred,
  aes(True, Predicted)) +
  geom_point() +
  geom_abline(int = 0, sl = 1,
    col = 'darkgray') +
  facet_grid(~ Component)
```



The prediction of the Permanent Environmental Competition effect is not precisely great...

Competition #2 | Map of residuals and their variogram

```
plot(res.comp, type = 'resid')
variogram(res.comp)
```



Generic component

This additional component allows to introduce a random effect ψ with **arbitrary** incidence and covariance matrices Z and Σ :

$$y = \mu + X\beta + Z\psi + \varepsilon$$

$$\psi \sim N(0, \sigma_\psi^2 \Sigma_\psi)$$

$$\varepsilon \sim N(0, \sigma_\varepsilon^2)$$

```
## Fit a blocks effect using generic
inc.mat <- model.matrix(~ 0 + bl, globulus)
cov.mat <- diag(nlevels(globulus$bl))
res.blg <- remlf90(fixed = phe_X ~ gg,
                   generic = list(block = list(inc.mat,
                                                cov.mat)),
                   data = globulus)
```

```
summary(res.blg)
```

```
## Linear Mixed Model with pedigree and spatial effects fit by AI-REMLF90 ver. 1.122
##   Data: globulus
##   AIC  BIC logLik
## 5691 5701 -2844
##
## Parameters of special components:
```

```
##
##
## Variance components:
##           Estimated variances   S.E.
## block                2.592 1.0640
## Residual              15.208 0.6825
##
## Fixed effects:
##           value   s.e.
## gg.1  13.534 0.6222
## gg.2  14.030 0.8464
## gg.3  16.106 0.5513
## gg.4  11.854 0.6824
## gg.5  15.883 0.5863
## gg.6  10.220 1.3041
## gg.7  13.995 1.0894
## gg.8  15.728 0.5410
## gg.9  16.478 0.5969
## gg.10 12.843 1.1225
## gg.11 16.744 0.6151
## gg.12 17.002 0.8464
## gg.13 16.297 1.0894
## gg.14 14.429 0.4730
```

Prediction

Predicting values for unobserved trees

- You can predict the Breeding Value of an **unmeasured tree**
- Or the expected phenotype of a death tree (or an hypothetical scenario)
- Information is gathered from the covariates, the spatial structure and the pedigree
- Simply **include the individual** in the dataset with the response set as NA

Leave-one-out cross-validation

- Re-fit the simulated competition data with one measurement removed
- Afterwards, compare the predicted values for the **unmeasured** individuals with their true simulated values

```
rm.idx <- 8
rm.exp <- with(dat[rm.idx, ],
               phenotype - resid)
dat.loo <- dat
dat.loo[rm.idx, 'phenotype'] <- NA
```

	True	Pred.loo
direct BV	-1.48	0.11
competition BV	0.46	0.36
exp. phenotype	6.80	9.90

Exercise | Cross validation

1. Extend the last table to include the predicted value when the phenotype is measured
2. Remove 1/10th of the phenotypes randomly, and predict their expected phenotype
 - Have the parameter estimations changed too much?
3. Compute the Root Mean Square Error (RMSE) of Prediction with respect to the true values

Cross-validation #1 | Include prediction with full data

```
pred.BV.mat <- with(ranef(res.comp), cbind(`genetic_direct`,
                                          `genetic_competition`))

pred.genetic.loo <-
  Zd[rm.idx, ] %%% with(ranef(res.comp),
                        cbind(`genetic_direct`,
                              `genetic_competition`))
valid.pred$Pred.full <- c(Zd[rm.idx, ] %%% pred.BV.mat,
                          fitted(res.comp)[rm.idx])

knitr::kable(round(valid.pred[,c(1,3,2)],
                    2))
```

	True	Pred.full	Pred.loo
direct BV	-1.48	-1.30	0.11
competition BV	0.46	0.99	0.36
exp. phenotype	6.80	7.29	9.90

Cross-validation #2 | Perform cross-validation on 1/10th of the observations

```
rm.idx <- sample(nrow(dat),
                 nrow(dat)/10)
dat.cv <- dat
dat.cv[rm.idx, 'phenotype'] <- NA
## Re-fit the model and build table
```

	Fully.estimated	CV.estimated
direct	2.50	2.69
compet.	1.03	0.86
correl.	-0.76	-0.80
spatial	1.24	1.03
pec	0.20	0.51
residual	0.17	0.14

Cross-validation #3 | MSE of Prediction

```
true.exp.cv <- with(dat[rm.idx, ], phenotype - resid)
round(sqrt(mean((fitted(res.comp.cv)[rm.idx] - true.exp.cv)^2)), 2)
```

```
## [1] 1.5
```

Some more features

Metagene interface

- We have used simulated data from the `metagene` software
- If you simulate data, import the results with `read.metagene()`
- Use several common methods with a `metagene` object:
 - `summary()`, `plot()`, `as.data.frame()`
- Plus some more specific `metagene` functions:
 - `b.values()`, `get.ntraits()`, `ngenerations()`, `nindividuals()`, `get.pedigree()`
- And specific functions about spatial arrangement:
 - `coordinates()` extract coordinates
 - `sim.spatial()` simulates some spatial autocorrelation

Simulation framework

- The function `breedR.sample.phenotype()` simulates datasets from all the model structures available in **breedR**
- Limitation: only one generation, with random matings of founders
- See `?simulation` for details

Remote computation

If you have access to a **Linux** server through **SSH**, you can perform computations remotely

- Take advantage of more **memory** or **faster** processors
- **Parallelize** jobs
- Free **local resources** while fitting models
- See `?remote` for details

Package options

- **breedR** features a list of configurable options
- Use `breedR.setOption(...)` for changing an option during the current session
- Set options permanently in the file `$HOME/.breedRrc`
- see `?breedR.option` for details

```
breedR.getOption()
```

```
## $ar.eval
## [1] -0.8 -0.2  0.2  0.8
##
## $breedR.bin
## [1] "/home/facu/Work/Proyectos/2013.T4F/bin/PROGSF90/linux/32bit"
##
## $splines.nok
## determine.n.knots
##
## $default.initial.variance
## [1] 1
##
## $col.seq
## [1] "#034E7B" "#FDAE6B"
##
## $col.div
## [1] "#3A3A98FF" "#832424FF"
##
## $cygwin
## [1] "C:/cygwin"
##
## $cygwin.home
## [1] "/home/facu"
##
## $ssh.auth.sock
## [1] "/tmp/ssh-auth-sock-facu"
##
## $remote.host
## [1] "eldorado"
##
## $remote.user
## [1] "fmunoz"
##
## $remote.port
## [1] 22
##
## $remote.bin
## [1] "/home/fmunoz/R/x86_64-unknown-linux-gnu-library/3.0/breedR/bin/linux"
##
## $ssh.options
## [1] "-x -o BatchMode=yes -o TCPKeepAlive=yes -e none"
```