Understanding variance-covariance structures - simple and more complex

Objectives:

- Introduce the direct product operator ⊗ for variance-covariance structures *V*
- Show how simple variance-component models can be formulated using ⊗
- Show how more complex models can be formulated using ⊗

Why?

- Because ASReml-R uses this formulation
- You can't intelligently talk to ASReml-R without being familiar with this operator

General formulation of mixed model

$$y = X\beta + Zu + e$$

with

$e \sim \mathrm{MNV}(0,R)$,

$u \sim \mathrm{MNV}(0,G)$, and

$y \sim \mathrm{MNV}(X\beta, V)$, where $V = ZGZ^T + R$.

Best Linear Unbiased Estimation (BLUE)

$$\hat{\beta} = \left(X^T V^{-1} X\right)^{-} X^T V^{-1} y$$

Best Linear Unbiased Prediction (BLUP)

$$u = G Z^T V^{-1}\left(y - X\hat{\beta}\right)$$

Mixed Model Equations (MME)

$$\begin{pmatrix} X^T R^{-1} X & X^T R^{-1} Z \\ Z^T R^{-1} X & Z^T R^{-1} Z + G^{-1} \end{pmatrix} \begin{pmatrix} \hat{\beta} \\ \hat{u} \end{pmatrix} = \begin{pmatrix} X^T R^{-1} y \\ Z^T R^{-1} y \end{pmatrix} ,$$

$\Rightarrow$ yield BLUE and BLUP simultaneously

Kronecker product

= direct product = tensor product

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & a_{13}B \\ a_{21}B & a_{22}B & a_{23}B \\ a_{31}B & a_{32}B & a_{33}B \end{pmatrix}$$

Some useful facts about Kronecker products

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$$

$$(A \otimes B)(C \otimes D) = AC \otimes BD$$

Randomized complete block design

$$y_{ij} = \mu + g_i + b_j + e_{ij}$$

Y = GEN + BLOCK : BLOCK•PLOT

Treatment model

Block model

$$\text{var}(b_j) = \sigma_b^2$$

$$\text{var}(e_{ij}) = \sigma_e^2$$

Matrix formulation

$$y = X\beta + Zu + e$$

Example:

r = number of complete blocks (replicates) = 2

k = number of plots per block = 12

$$u = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \quad , \ \mathrm{var}(u) = G = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \sigma_b^2 = I_r \sigma_b^2 \quad , \ Z = \begin{pmatrix} 1_{12} & 0_{12} \\ 0_{12} & 1_{12} \end{pmatrix} = I_r \otimes 1_k$$

$$\mathrm{var}(Zu) = ZGZ^T = \left(I_r \otimes 1_k\right)\Big|\left(I_r \otimes 1\right)\sigma_b^2\left(I_r \otimes 1_k^T\right)\Big| = I_r \otimes 1_k 1_k^T \sigma_b^2 = I_r \otimes J_k \sigma_b^2$$

Some basic matrices defined

A vector of n ones:

$$1_n = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ \vdots \\ 1 \end{pmatrix}$$

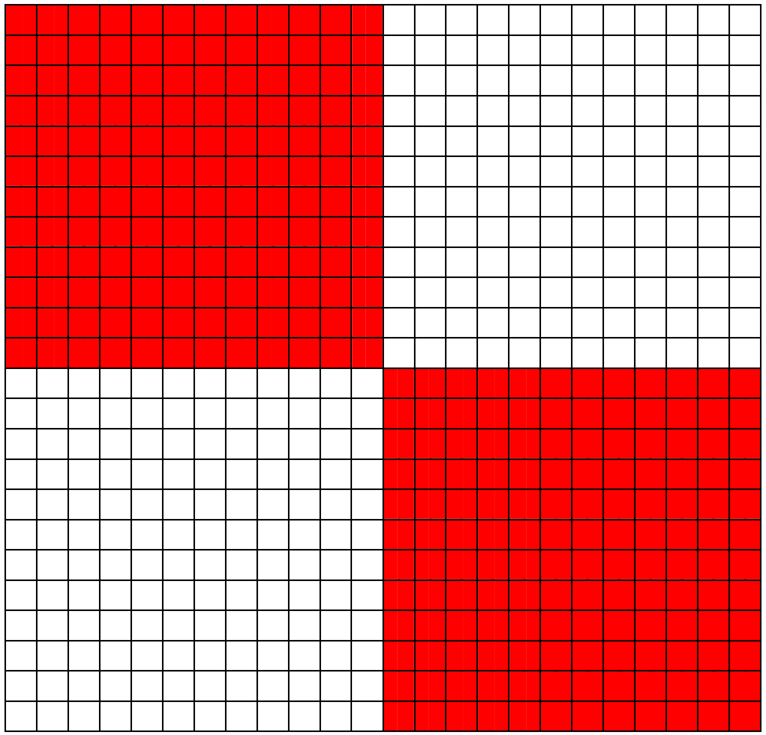
An identity matrix: n ones on diagonal

$$I_n = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & & & 0 \\ \vdots & & 1 & & \vdots \\ 0 & & & \ddots & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}$$

An $n \times n$ matrix of ones everywhere

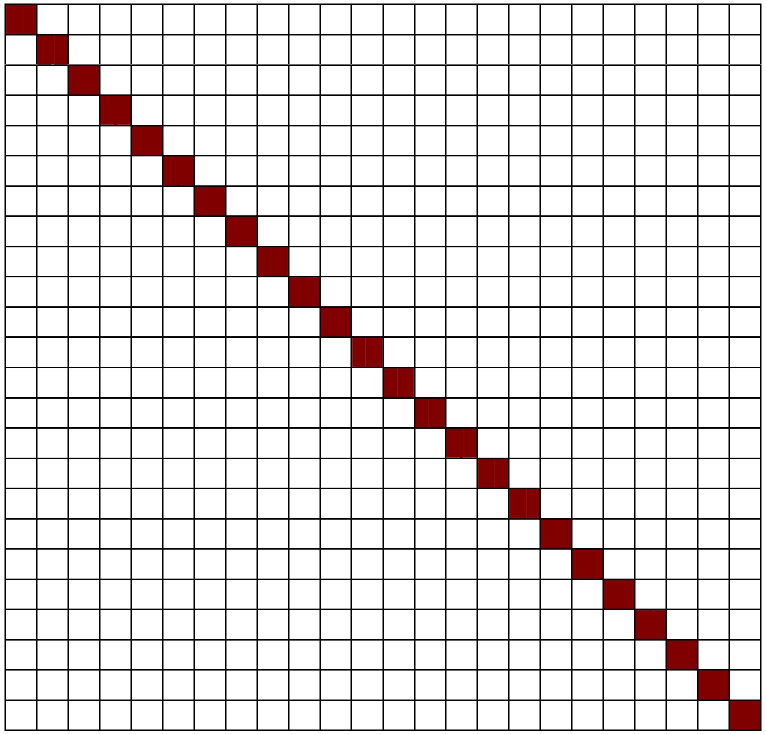
$$J_n = \begin{pmatrix} 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & & & 1 \\ \vdots & & 1 & & \vdots \\ 1 & & & \ddots & 1 \\ 1 & 1 & \cdots & 1 & 1 \end{pmatrix}$$

$$\operatorname{var}(Zu) = I_r \otimes J_k \sigma_b^2 = I_2 \otimes J_{12} \sigma_b^2 = \begin{pmatrix} J_{12} & 0 \\ 0 & J_{12} \end{pmatrix} \sigma_b^2 =$$



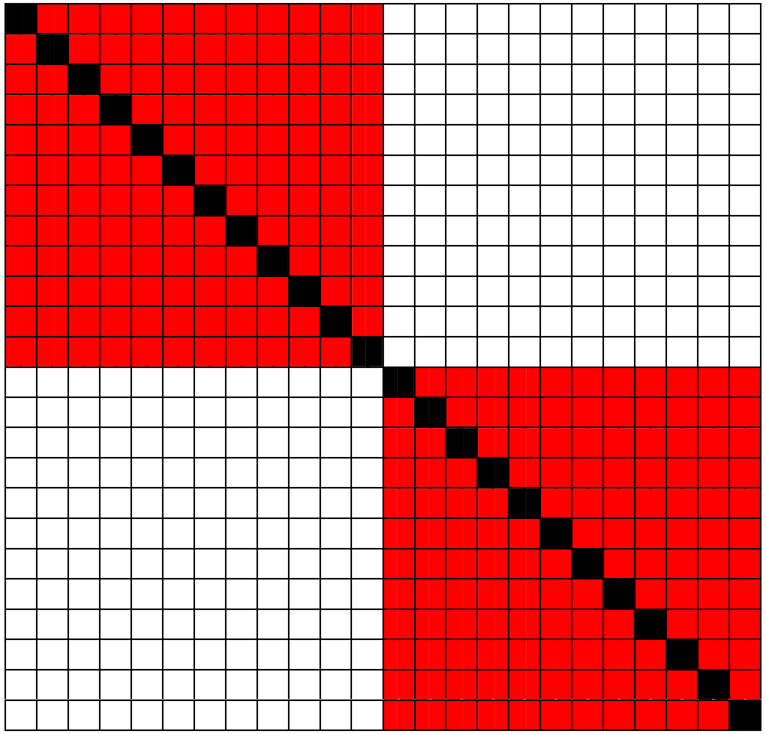
σ_b^2

$$\operatorname{var}(e) = I_r \otimes I_k \sigma_e^2 = I_{rk} \sigma_e^2 = I_{24} \sigma_e^2$$



σ_e^2

$$\mathrm{var}(Zu+e) = I_r \otimes J_k\sigma_b^2 + I_r \otimes I_k\sigma_e^2 = I_r \otimes \left(J_k\sigma_b^2 + I_k\sigma_e^2\right)$$



(red)	σ_b^2	Covariance among plots in the same block
(black)	$\sigma_b^2 + \sigma_e^2$	Variance of an observation

Resolvable incomplete block design (α-design)

Replicate 1				Replicate 2			
1	2	3		1	2	3	Block no.
4	7	8		4	9	5	
10	3	1		12	8	3	
2	12	5		11	7	2	
6	11	9		1	10	6	

plot

incomplete block

replicate

Block model:

REP/BLOCK/PLOT = REP : REP•BLOCK + <u>REP•BLOCK•PLOT</u>

$$y_{ijh} = \mu + g_i + \gamma_j + b_{jh} + e_{ijh}$$

Y = GEN : REP/BLOCK/PLOT

Matrix formulation

$$y = X\beta + Z_1 u_1 + Z_2 u_2 + e$$

Here:

$$u_1 = \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix},\ \mathrm{var}(u_1) = G_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\sigma_\gamma^2 = I_r\sigma_r^2,\ Z_1 = \begin{pmatrix} 1_{12} & 0_{12} \\ 0_{12} & 1_{12} \end{pmatrix} = I_r \otimes 1_b \otimes 1_k$$

r = number of replicates = 2

b = number of incomplete blocks per replicate = 3

k = number of plots per block = 4

$$\mathrm{var}(Z_1 u_1) = Z_1 G_1 Z_1^T = (I_r \otimes 1_b \otimes 1_k)\Big|(I_r \otimes 1 \otimes 1)\sigma_r^2 (I_r \otimes 1_b^T \otimes 1_k^T)\Big| = I_r \otimes J_b \otimes J_k \sigma_\gamma^2$$

Here:

$$u_2 = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{21} & b_{22} & b_{23} \end{pmatrix}^T,\ \mathrm{var}(u_2) = I_r \otimes I_b \sigma_b^2,\ Z_2 = I_r \otimes I_b \otimes 1_k$$

r = number of replicates = 2

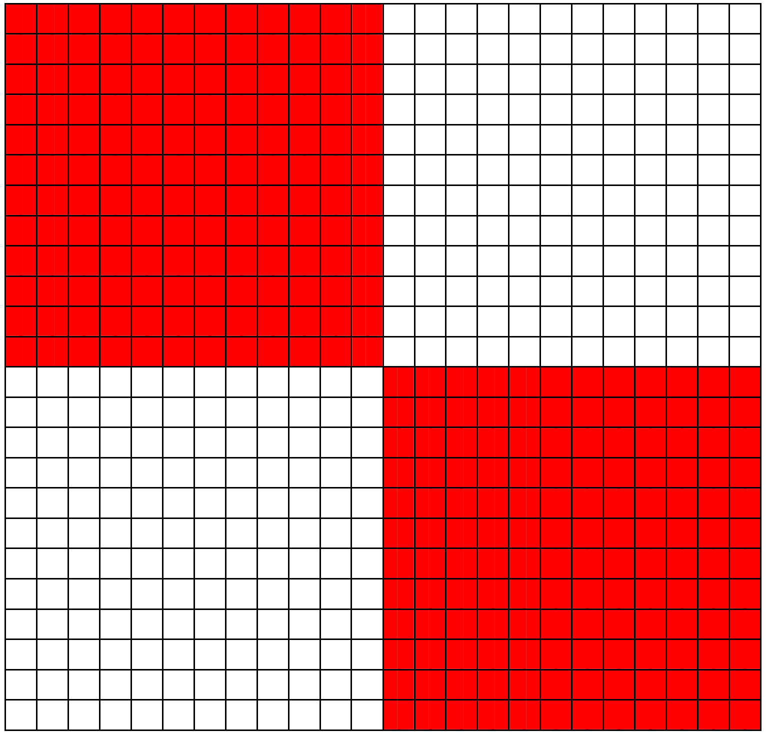
b = number of incomplete blocks per replicate = 3

k = number of plots per block = 4

$$\mathrm{var}(Z_2 u_2) = Z_2 G_2 Z_2^T = (I_r \otimes I_b \otimes 1_k)(I_r \otimes I_b \otimes 1)\sigma_b^2 (I_r \otimes I_b \otimes 1_k^T) = I_r \otimes I_b \otimes J_k \sigma_b^2$$

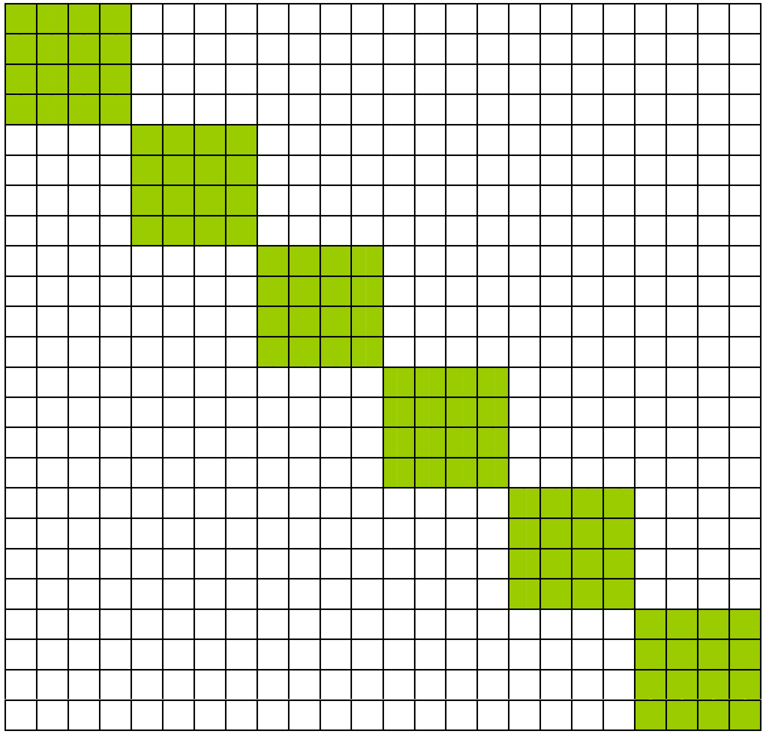
$$\mathrm{var}(Z_1 u_1 + Z_2 u_2 + e) = I_r \otimes J_b \otimes J_k \sigma_\gamma^2 + I_r \otimes I_b \otimes J_k \sigma_b^2 + I_r \otimes I_b \otimes I_k \sigma_e^2$$

$$\mathrm{var}(Z_1 u_1) = I_r \otimes J_b \otimes J_k \sigma_\gamma^2$$



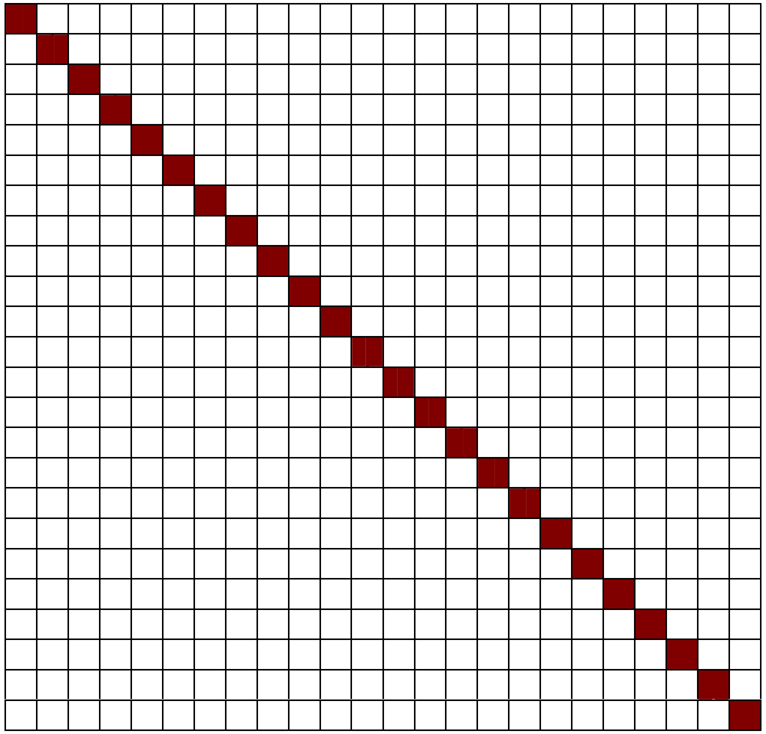
σ_γ^2

$$\mathrm{var}(Z_2 u_2) = I_r \otimes I_b \otimes J_k \sigma_b^2$$



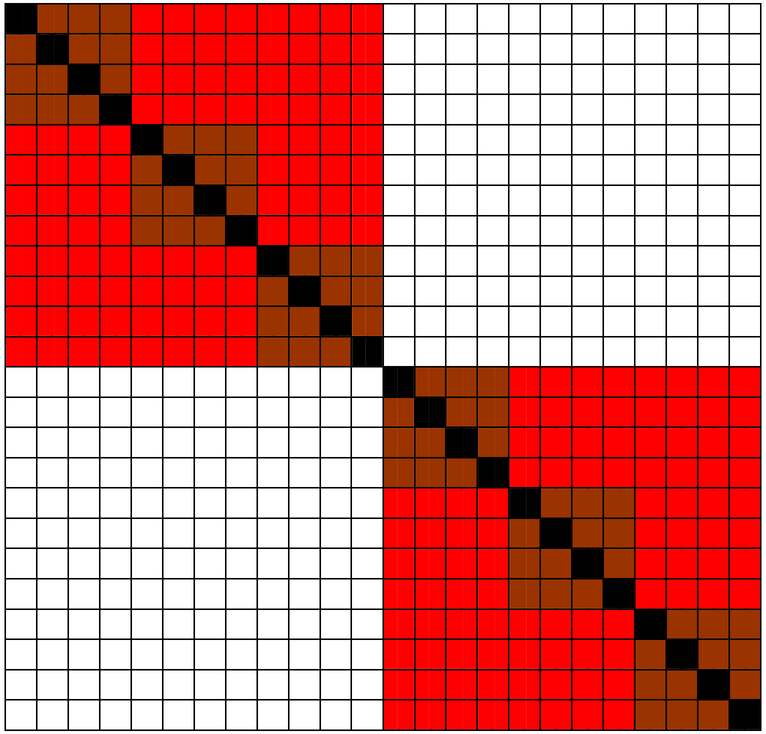
σ_b^2

$$\mathrm{var}(e) = I_r \otimes I_b \otimes I_k \sigma_e^2$$



 σ_e^2

$$\mathrm{var}(Z_1u_1 + Z_2u_2 + e) = I_r \otimes J_b \otimes J_k\sigma_\gamma^2 + I_r \otimes I_b \otimes J_k\sigma_b^2 + I_r \otimes I_b \otimes I_k\sigma_e^2$$



(red)	σ_γ^2	Covariance among plots in same rep, but different block
(brown)	$\sigma_\gamma^2 + \sigma_b^2$	Covariance among plots in the same block
(black)	$\sigma_\gamma^2 + \sigma_b^2 + \sigma_e^2$	Variance of an observation

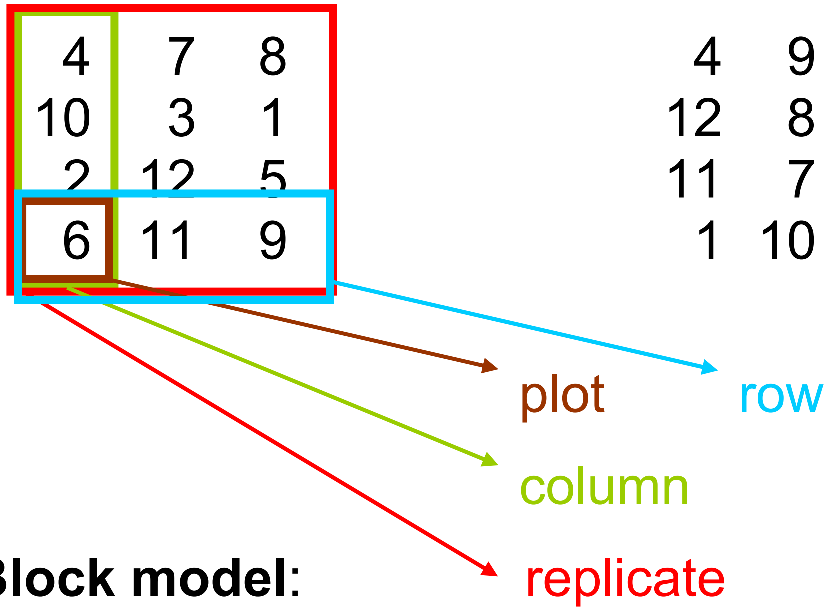
Resolvable row-column design

Replicate 1

1	2	3
4	7	8
10	3	1
2	12	5
6	11	9

Replicate 2

1	2	3
4	9	5
12	8	3
11	7	2
1	10	6



Block model:

$$REP/(ROW \times COL) = REP + REP \bullet ROW + REP \bullet COL + \underline{REP \bullet ROW \bullet COL}$$

$$y_{ijhk} = \mu + g_i + \gamma_j + r_{jh} + c_{jk} + e_{ijhk}$$

Y = GEN : REP/(ROW×COL)

Matrix formulation

$y = X\beta + Z_1 u_1 + Z_2 u_2 + Z_3 u_3 + e$

Here:

$$u_1 = \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix},\ \mathrm{var}(u_1) = G_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \sigma_\gamma^2 = I_r \sigma_r^2,\ Z_1 = \begin{pmatrix} 1_{12} & 0_{12} \\ 0_{12} & 1_{12} \end{pmatrix} = I_r \otimes 1_b \otimes 1_k$$

r = number of replicates = 2

s = number of columns per replicate = 3

k = number of rows per block = 4

$$\mathrm{var}(Z_1 u_1) = Z_1 G_1 Z_1^T = (I_r \otimes 1_b \otimes 1_k)(I_r \otimes 1 \otimes 1)\sigma_r^2 (I_r \otimes 1_b^T \otimes 1_k^T) = I_r \otimes J_b \otimes J_k \sigma_\gamma^2$$

Here:

$$u_2 = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{21} & c_{22} & c_{23} \end{pmatrix}^T, \ \mathrm{var}(u_2) = I_r \otimes I_s \sigma_c^2, \ Z_2 = I_r \otimes I_s \otimes 1_k$$

r = number of replicates = 2

s = number of columns per replicate = 3

k = number of rows per replicate = 4

$$\mathrm{var}(Z_2 u_2) = Z_2 G_2 Z_2^T = (I_r \otimes I_s \otimes 1_k)(I_r \otimes I_s \otimes 1)\sigma_b^2 (I_r \otimes I_s \otimes 1_k^T) = I_r \otimes I_s \otimes J_k \sigma_b^2$$

$$\mathrm{var}(Z_1 u_1 + Z_2 u_2 + e) = I_r \otimes J_b \otimes J_k \sigma_\gamma^2 + I_r \otimes I_b \otimes J_k \sigma_b^2 + I_r \otimes I_b \otimes I_k \sigma_e^2$$

Here:

$$u_3 = \begin{pmatrix} r_{11} & r_{12} & r_{13} & r_{14} & r_{21} & r_{22} & r_{23} & r_{24} \end{pmatrix}^T, \ \mathrm{var}(u_3) = I_r \otimes I_k \sigma_r^2,$$
$$Z_3 = I_r \otimes 1_s \otimes I_k$$

r = number of replicates = 2

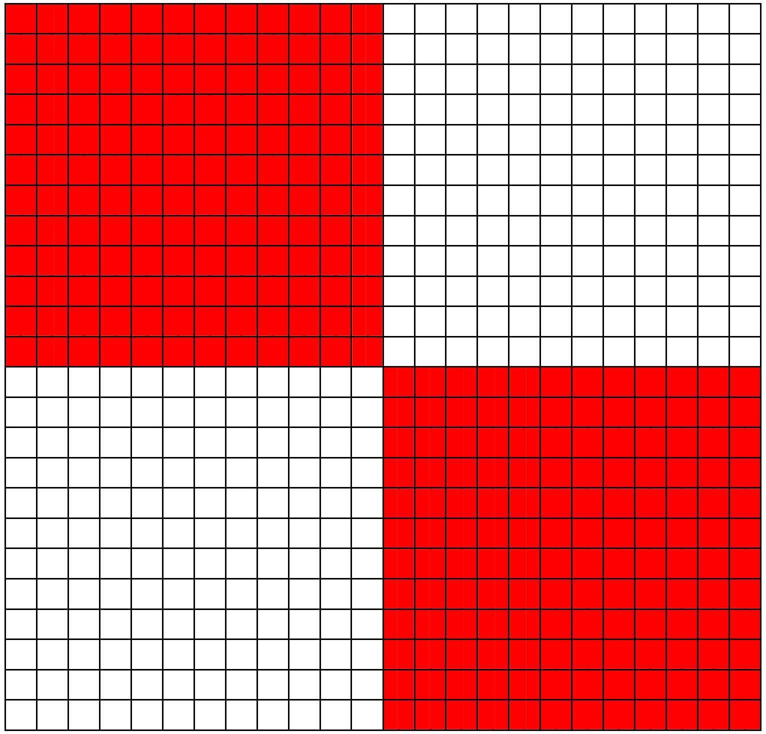
s = number of columns per replicate = 3

k = number of rows per replicate = 4

$$\mathrm{var}(Z_3 u_3) = Z_3 G_3 Z_3^T = (I_r \otimes 1_s \otimes I_k)(I_r \otimes 1 \otimes I_s)\sigma_r^2 (I_r \otimes 1_s^T \otimes I_k) = I_r \otimes J_s \otimes I_k \sigma_r^2$$

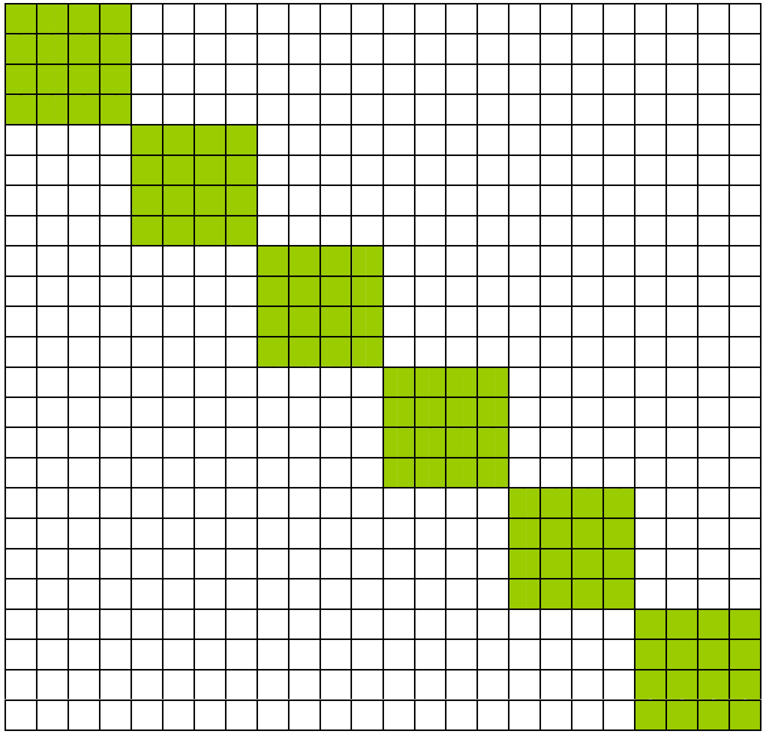
$$\mathrm{var}(Z_1 u_1 + Z_2 u_2 + Z_3 u_3 + e)$$
$$= I_r \otimes J_b \otimes J_k \sigma_\gamma^2 + I_r \otimes I_s \otimes J_k \sigma_c^2 + I_r \otimes J_s \otimes I_k \sigma_r^2 + I_r \otimes I_b \otimes I_k \sigma_e^2$$

$$\mathrm{var}(Z_1 u_1) = I_r \otimes J_b \otimes J_k \sigma_\gamma^2$$



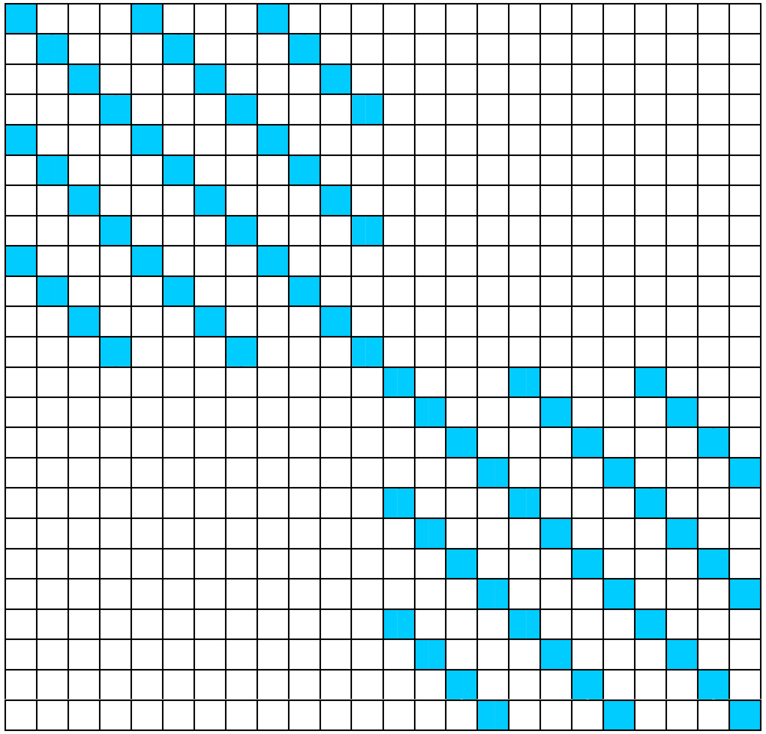
σ_γ^2

$$\mathrm{var}(Z_2 u_2) = I_r \otimes I_s \otimes J_k \sigma_c^2$$



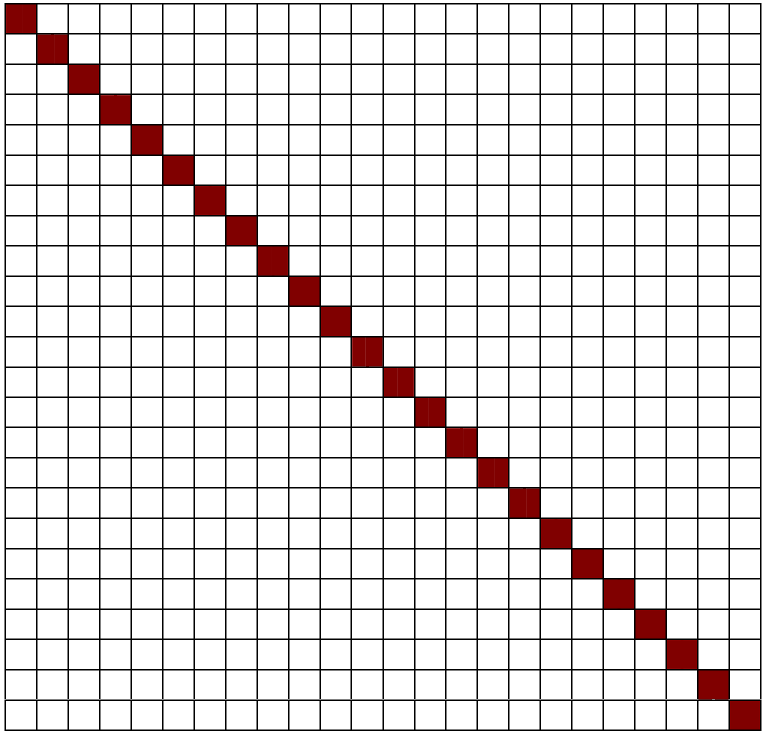
■ σ_c^2

$$\mathrm{var}(Z_3 u_3) = I_r \otimes J_s \otimes I_k \sigma_r^2$$



σ_r^2

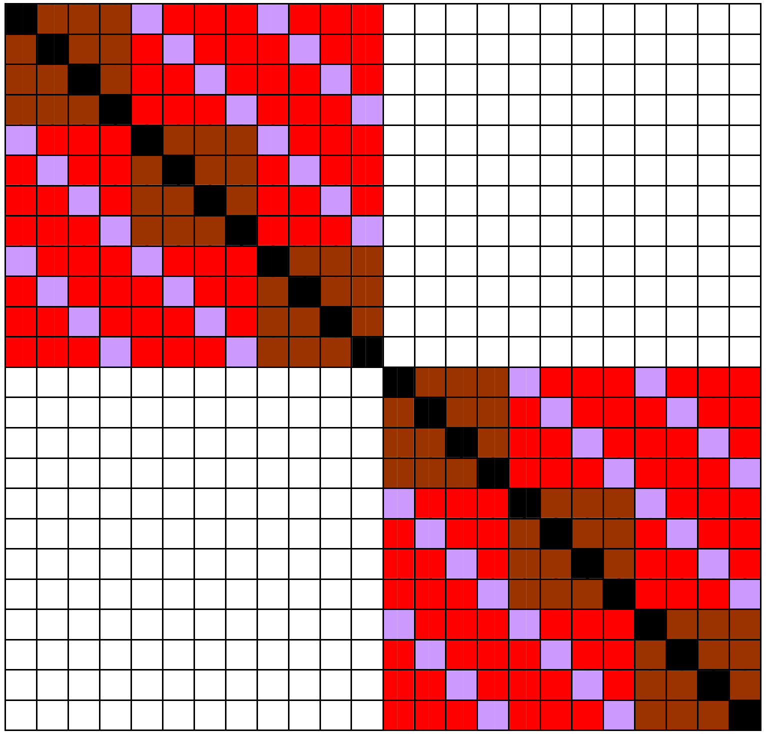
$$\operatorname{var}(e) = I_r \otimes I_b \otimes I_k \sigma_e^2$$



σ_e^2

$$\mathrm{var}(Z_1u_1 + Z_2u_2 + Z_3u_3 + e)$$

$$= I_r \otimes J_b \otimes J_k\sigma_\gamma^2 + I_r \otimes I_s \otimes J_k\sigma_c^2 + I_r \otimes J_s \otimes I_k\sigma_r^2 + I_r \otimes I_b \otimes I_k\sigma_e^2$$



σ_γ^2

$\sigma_\gamma^2 + \sigma_c^2$

$\sigma_\gamma^2 + \sigma_r^2$

$\sigma_\gamma^2 + \sigma_c^2 + \sigma_r^2 + \sigma_e^2$

More complex structures: A spatial model

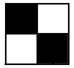
$$y_{ijhk} = \mu + g_i + \gamma_j + r_{jh} + c_{jk} + \boldsymbol{t_{ijhk}} + e_{ijhk}$$

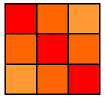
Y = GEN : REP/(ROW×COL)

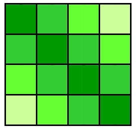
$$\mathrm{var}(t) = I_r \otimes \Omega_s \otimes \Omega_k \sigma_t^2$$

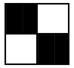
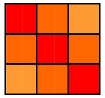
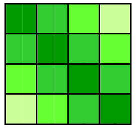
Ω_s = spatial correlation matrix for columns

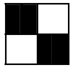
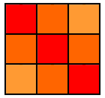
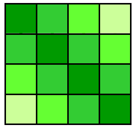
Ω_k = spatial correlation matrix for rows

$I_r =$ 

$\Omega_s =$ 

$\Omega_k =$ 

$I_r \otimes \Omega_s \otimes \Omega_k =$  $\otimes$  $\otimes$ 

$I_r \otimes \Omega_s \otimes \Omega_k =$  $\otimes$  $\otimes$ 

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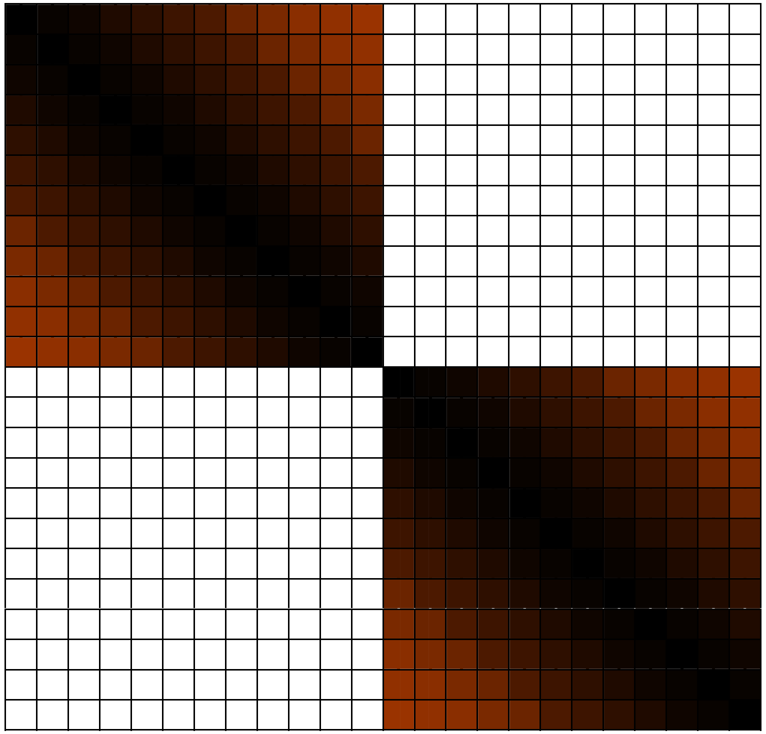


Coding in ASReml-R

Variables in dataframe:
REP = replicates
COL = columns
ROW = rows

$$I_r\sigma^2 \otimes \Omega_s \otimes \Omega_k$$

```
residual = ~idv(REP):ar1(COL):ar1(ROW)
```

Important: Data must be ordered by REP, COL and ROW

Linear variance (LV) (Williams, 1986)

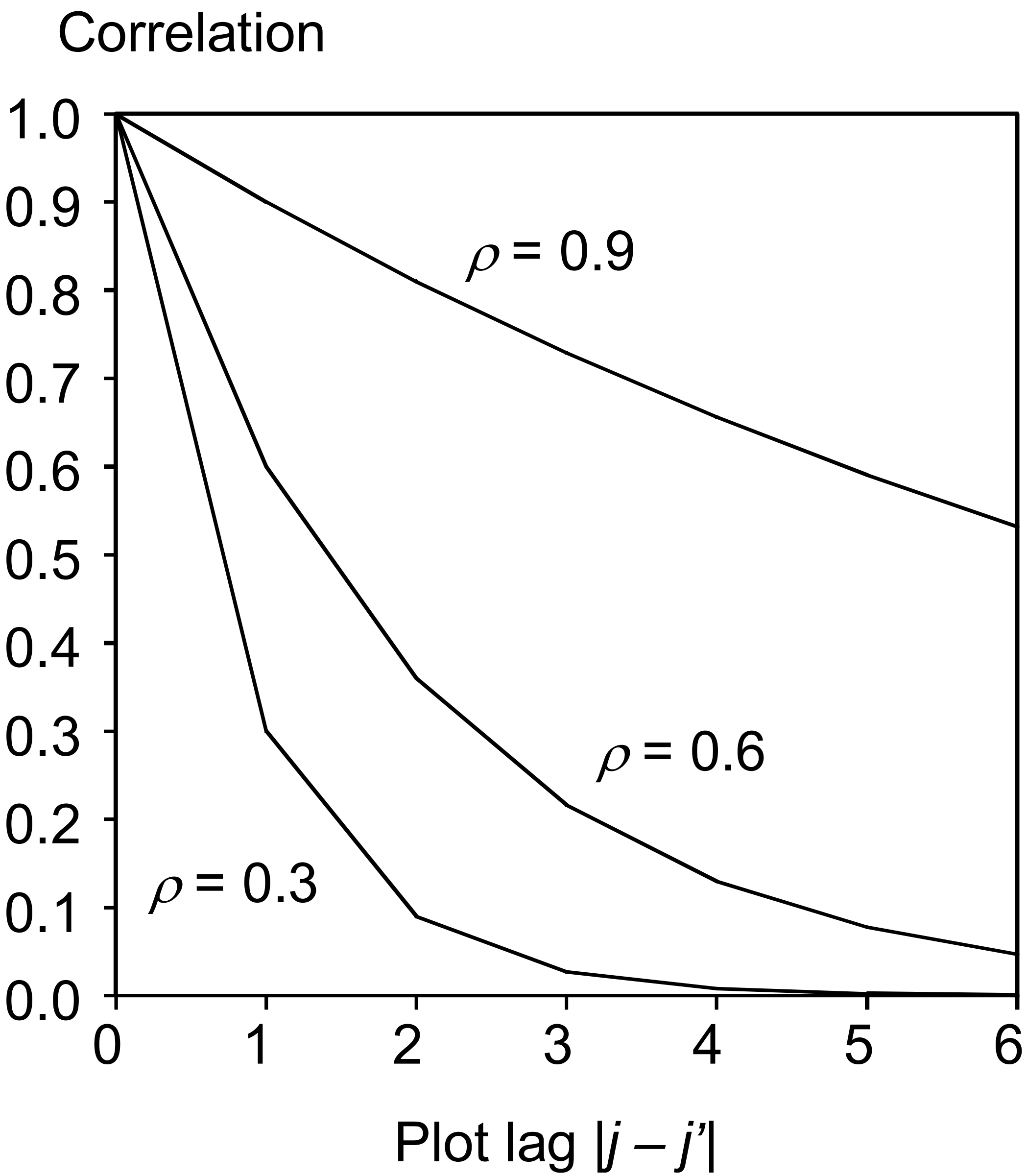
$$\text{cov}(t_1, t_2) = \sigma_t^2 (1 - \phi d),$$

t_1, t_2 = trend values on two plots

d = the distance of these two plots

AR(1) model

$$\text{cov}(t_1, t_2) = \sigma_t^2 \rho^d \quad (0 < \rho < 1)$$


Correlation
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
ρ = 0.9
ρ = 0.6
ρ = 0.3
0
1
2
3
4
5
6
Plot lag |j – j'|

AR(1) model

General class of spatial covariance model

$$\text{var}(t_1) = \text{var}(t_2) = \sigma_t^2$$

$$\text{cov}(t_1, t_2) = \sigma_t^2 f(d)$$

$f(d)$ is some smooth decreasing function of d with $f(0) = 1$.

Many other models: Gaussian, Spherical, etc.

Model diagnosis by semivariogram

Semivariance:

$$v = \frac{1}{2}(y_1 - y_2)^2$$

$$E(v) = \gamma(d) = \sigma_e^2 + \sigma_t^2\left[1 - f(d)\right]$$

σ_t^2 = variance of trend

σ_e^2 = nugget variance

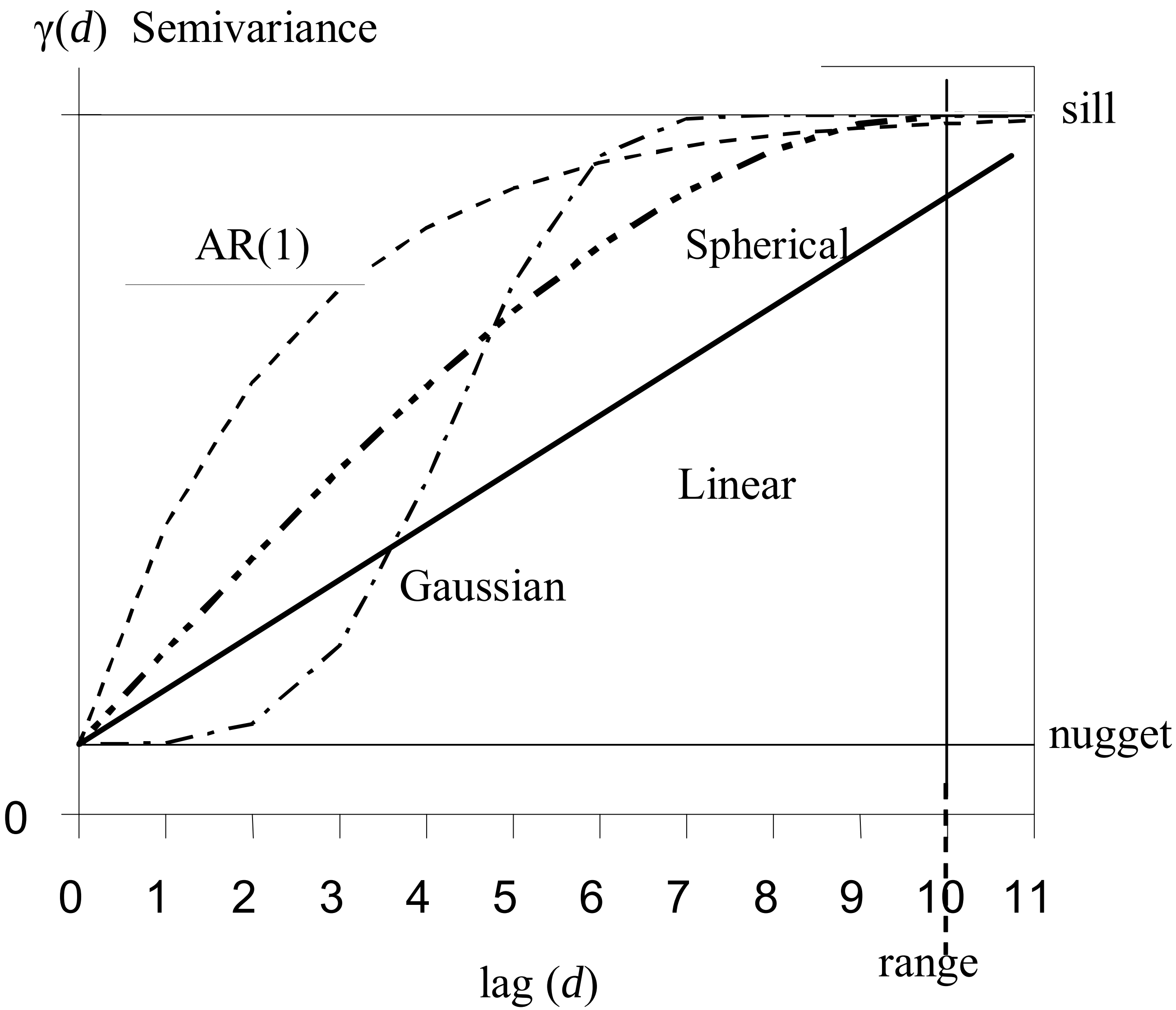


Fig.: Examples of some semi-variogram models.

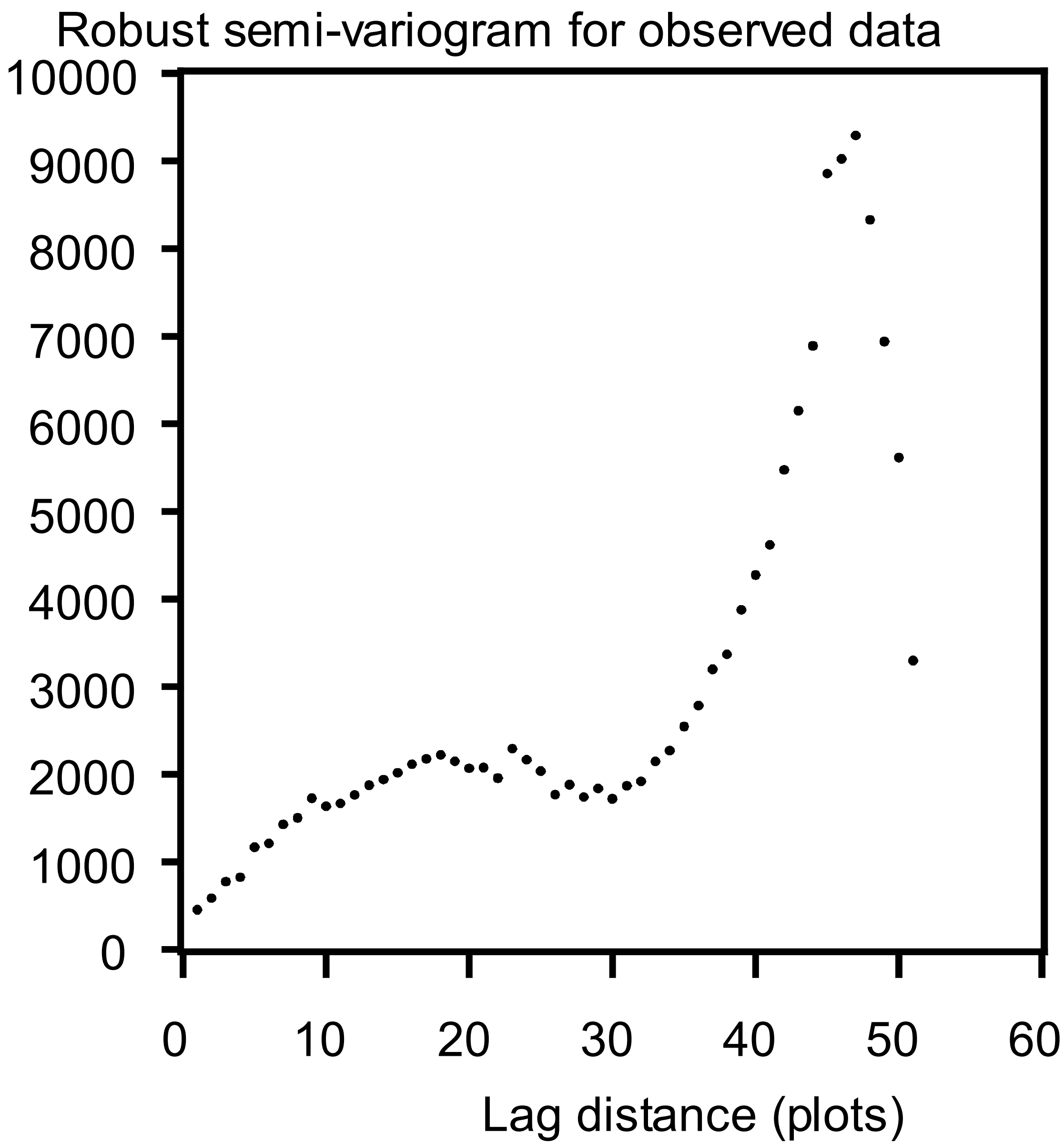


Fig 13: Robust semi-variogram for wheat data of Besag & Kempton (1986).

The AR(1) ⊗ AR(1) model

$$\mathrm{var}(t_i) = \sigma_t^2$$

$$\mathrm{cov}(t_i, t_j) = \sigma_t^2 \rho_C^{d_C} \rho_R^{d_R}$$

d_C = distance between plots i and j in column direction

d_R = distance between plots i and j in row direction

ρ_C = correlation between plots i and j in column direction

ρ_R = correlation between plots i and j in row direction

The model is **anisotropic** because correlation depends on direction

$$\text{cov}(t_i, t_j) = \sigma_t^2 \rho_C^{d_C} \rho_R^{d_R}$$

variance

correlation in column

correlation in row

Direct product structure

$$\Omega_s = \begin{pmatrix} 1 & \rho_C & \rho_C^2 \\ \rho_C & 1 & \rho_C \\ \rho_C^2 & \rho_C & 1 \end{pmatrix} \qquad \Omega_k = \begin{pmatrix} 1 & \rho_R & \rho_R^2 & \rho_R^3 \\ \rho_R & 1 & \rho_R & \rho_R^2 \\ \rho_R^2 & \rho_R & 1 & \rho_R \\ \rho_R^3 & \rho_R^2 & \rho_R & 1 \end{pmatrix}$$

$$\Omega_s \otimes \Omega_k = \begin{pmatrix} 1 & \rho_C & \rho_C^2 \\ \rho_C & 1 & \rho_C \\ \rho_C^2 & \rho_C & 1 \end{pmatrix} \otimes \Omega_k = \begin{pmatrix} \Omega_k & \rho_C\Omega_k & \rho_C^2\Omega_k \\ \rho_C\Omega_k & \Omega_k & \rho_C\Omega_k \\ \rho_C^2\Omega_k & \rho_C\Omega_k & \Omega_k \end{pmatrix}$$

Example

Plot A in row 1 and column 2

Plot B in row 4 and column 3

$$\Omega_s \otimes \Omega_k = \begin{pmatrix} 1 & \rho_C & \rho_C^2 \\ \rho_C & 1 & \rho_C \\ \rho_C^2 & \rho_C & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \rho_R & \rho_R^2 & \rho_R^3 \\ \rho_R & 1 & \rho_R & \rho_R^2 \\ \rho_R^2 & \rho_R & 1 & \rho_R \\ \rho_R^3 & \rho_R^2 & \rho_R & 1 \end{pmatrix}$$

This model is **separable**

It has separate structures for rows and columns

$$
\Omega_S \otimes \Omega_k = \begin{pmatrix}
1 & \rho_R & \rho_R^2 & \rho_R^3 & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_C\rho_R^3 & \rho_C^2 & \rho_C^2\rho_R & \rho_C^2\rho_R^2 & \rho_C^2\rho_R^3 \\
\rho_R & 1 & \rho_R & \rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_C^2\rho_R & \rho_C^2 & \rho_C^2\rho_R & \rho_C^2\rho_R^2 \\
\rho_R^2 & \rho_R & 1 & \rho_R & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_C^2\rho_R^2 & \rho_C^2\rho_R & \rho_C^2 & \rho_C^2\rho_R \\
\rho_R^3 & \rho_R^2 & \rho_R & 1 & \rho_C\rho_R^3 & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C^2\rho_R^3 & \rho_C^2\rho_R^2 & \rho_C^2\rho_R & \rho_C^2 \\
\rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_C\rho_R^3 & 1 & \rho_R & \rho_R^2 & \rho_R^3 & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_C\rho_R^3 \\
\rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_R & 1 & \rho_R & \rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 \\
\rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_R^2 & \rho_R & 1 & \rho_R & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R \\
\rho_C\rho_R^3 & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_R^3 & \rho_R^2 & \rho_R & 1 & \rho_C\rho_R^3 & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C \\
\rho_C^2 & \rho_C^2\rho_R & \rho_C^2\rho_R^2 & \rho_C^2\rho_R^3 & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_C\rho_R^3 & 1 & \rho_R & \rho_R^2 & \rho_R^3 \\
\rho_C^2\rho_R & \rho_C^2 & \rho_C^2\rho_R & \rho_C^2\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_C\rho_R^2 & \rho_R & 1 & \rho_R & \rho_R^2 \\
\rho_C^2\rho_R^2 & \rho_C^2\rho_R & \rho_C^2 & \rho_C^2\rho_R & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_C\rho_R & \rho_R^2 & \rho_R & 1 & \rho_R \\
\rho_C^2\rho_R^3 & \rho_C^2\rho_R^2 & \rho_C^2\rho_R & \rho_C^2 & \rho_C\rho_R^3 & \rho_C\rho_R^2 & \rho_C\rho_R & \rho_C & \rho_R^3 & \rho_R^2 & \rho_R & 1
\end{pmatrix}
$$

More complex structures: Kinship

α-design:

$$y_{ijh} = \mu + g_i + \gamma_j + b_{jh} + e_{ijh}$$

Y = GEN : REP/BLOCK/PLOT

$$g = \begin{pmatrix} g_1 \\ g_2 \\ \vdots \\ \vdots \\ g_v \end{pmatrix}$$

Independent genotypes

$$\text{var}(g) = I_v \sigma_g^2$$

v = number of genotypes

Kinship

$$\text{var}(g) = K_v \sigma_g^2$$

K_v = kinship matrix

More complex structures: multi-trait model

Three traits: A, B, C

$$g_A = \begin{pmatrix} g_{A1} \\ g_{A2} \\ \vdots \\ \vdots \\ g_{Av} \end{pmatrix} \qquad g_B = \begin{pmatrix} g_{B1} \\ g_{B2} \\ \vdots \\ \vdots \\ g_{Bv} \end{pmatrix} \qquad g_C = \begin{pmatrix} g_{C1} \\ g_{C2} \\ \vdots \\ \vdots \\ g_{Cv} \end{pmatrix} \qquad \Rightarrow \qquad g = \begin{pmatrix} g_A \\ g_B \\ g_C \end{pmatrix}$$

$$\text{var}(g_A) = \sigma_A^2 I_v \quad \text{var}(g_B) = \sigma_B^2 I_v \quad \text{var}(g_C) = \sigma_C^2 I_v$$

Covariances

$$\operatorname{cov}(g_A, g_B) = \sigma_{AB} I_v$$

$$\operatorname{cov}(g_A, g_C) = \sigma_{AC} I_v$$

$$\operatorname{cov}(g_B, g_C) = \sigma_{BC} I_v$$

Plug it all together:

$$\operatorname{var}(g) = \begin{pmatrix} \sigma_A^2 & \sigma_{AB} & \sigma_{AC} \\ \sigma_{BA} & \sigma_B^2 & \rho_{BC} \\ \sigma_{CA} & \rho_{CB} & \sigma_C^2 \end{pmatrix} \otimes I_v = \Sigma \otimes I_v$$

More complex structures: multi-trait model with kinship matrix $\boldsymbol{K_v}$

Three traits: A, B, C

$$g_A = \begin{pmatrix} g_{A1} \\ g_{A2} \\ \vdots \\ \vdots \\ g_{Av} \end{pmatrix} \qquad g_B = \begin{pmatrix} g_{B1} \\ g_{B2} \\ \vdots \\ \vdots \\ g_{Bv} \end{pmatrix} \qquad g_C = \begin{pmatrix} g_{C1} \\ g_{C2} \\ \vdots \\ \vdots \\ g_{Cv} \end{pmatrix} \qquad \Rightarrow \qquad g = \begin{pmatrix} g_A \\ g_B \\ g_C \end{pmatrix}$$

$$\mathrm{var}(g_A) = \sigma_A^2 K_v \qquad \mathrm{var}(g_B) = \sigma_B^2 K_v \qquad \mathrm{var}(g_C) = \sigma_C^2 K_v$$

Covariances

$$\mathrm{cov}(g_A, g_B) = \sigma_{AB} K_v$$

$$\mathrm{cov}(g_A, g_C) = \sigma_{AC} K_v$$

$$\mathrm{cov}(g_B, g_C) = \sigma_{BC} K_v$$

Plug it all together:

$$\mathrm{var}(g) = \begin{pmatrix} \sigma_A^2 & \sigma_{AB} & \sigma_{AC} \\ \sigma_{BA} & \sigma_B^2 & \rho_{BC} \\ \sigma_{CA} & \rho_{CB} & \sigma_C^2 \end{pmatrix} \otimes K_v = \Sigma \otimes K_v$$

Sigma and Gamma parameterizations

$$y = X\beta + Zu + e$$

with

$$e \sim \mathrm{MNV}(0, R)$$

$$u \sim \mathrm{MNV}(0, G)$$

$y \sim \mathrm{MNV}(X\beta, V)$, where $V = ZGZ^T + R$

$Zu = Z_1 u_1 + Z_2 u_2 + \ldots$ with $\mathrm{var}(u_i) = G_i$

For example: $\mathrm{var}(u_i) = G_i = I\sigma_{u_i}^2$ and $\mathrm{var}(e) = R = I\sigma_e^2$

Sigma-parameterization:

$$V = Z_1 G_1 Z_1^T \sigma_{u_1}^2 + Z_2 G_2 Z_2^T \sigma_{u_2}^2 + \ldots + I\sigma_e^2$$

Gamma-parameterization:

$$V = \sigma_e^2 \left(Z_1 G_1 Z_1^T \gamma_{u_1} + Z_2 G_2 Z_2^T \gamma_{u_1} + \ldots + I \right)$$ with $\gamma_{u_i} = \sigma_{u_i}^2 / \sigma_e^2$

General variance-covariance structure for factorial effect

Effect A•B•C•D•.....

$$Z_i G_i Z_i^T = \sigma_e^2 \left[\Omega_A(\gamma_A) \otimes \Omega_B(\gamma_B) \otimes \Omega_C(\gamma_C) \otimes \Omega_D(\gamma_D) \otimes \ldots \right]$$

This variance-covariance structure is **separable** for factors A, B, C, D, ...

Separability

$$\Omega_{u_{AB}} = \Omega_A \otimes \Omega_B =$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$\mathrm{corr}(u_{21}, u_{32}) = a_{23} \times b_{12}$$