

Nearest-Neighbor Analyses for field trials

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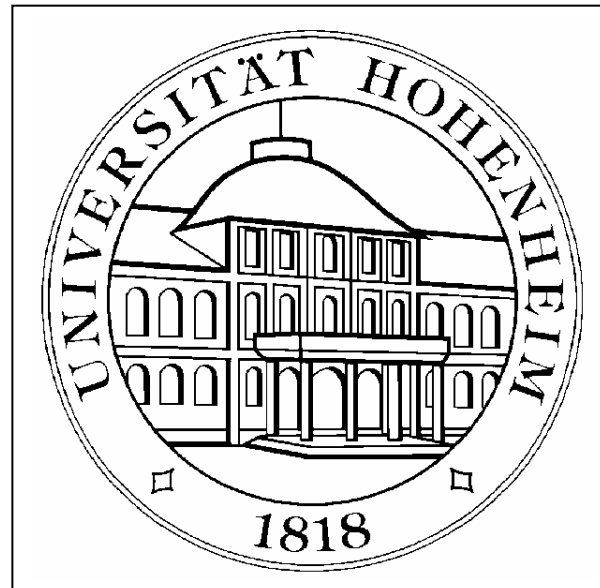


Table of contents

- 1. Introduction**
- 2. Nearest neighbour methods**
- 3. Linear variance models**
- 4. Nugget-Variogram**
- 5. Examples from field experiments**
- 6. Summary**

1. Introduction

Crop variety trials and plant breeding trials:

- Test performance for [target region](#)
- Trials in [large number of environments](#) (ideally random sample)

Standard trial designs for large number of treatments:

- Lattice designs, α -designs, row-column designs ([Williams and John, 1995](#))
- Designs with spatial analysis in mind ([Cullis et al., 2006](#); [Williams et al., 2006](#))

Background of our work:

- Variety and breeding trials laid out in classical incomplete blocks
- Need robust methods for routine use that exploits spatial correlation
- Old software very popular (ANOFT) \Rightarrow Need to switch to up-to-date software

Approaches for spatial analysis of field trials

(1) Fit a geostatistical model by default

Small-scale spatial trends: Stationary geostatistical models (default)

Large-scale trends: Polynomials, splines (add-on)

Extraneous variation: row and column effects (add-on)
(Serpentine harvesting of plots, multi-plot seeders, tractor reeling)

Model selection: Variogram inspection, likelihood-based inference (AIC)

(Gilmour et al., 1997)

(2) Fit a block model by default

- Use efficient resolvable incomplete block design or row-column design. Block effects (row and column effects) account for **large-scale trends** and **extraneous variation**
- Explore spatial correlation within blocks only as an add-on component (**small-scale spatial trends**)

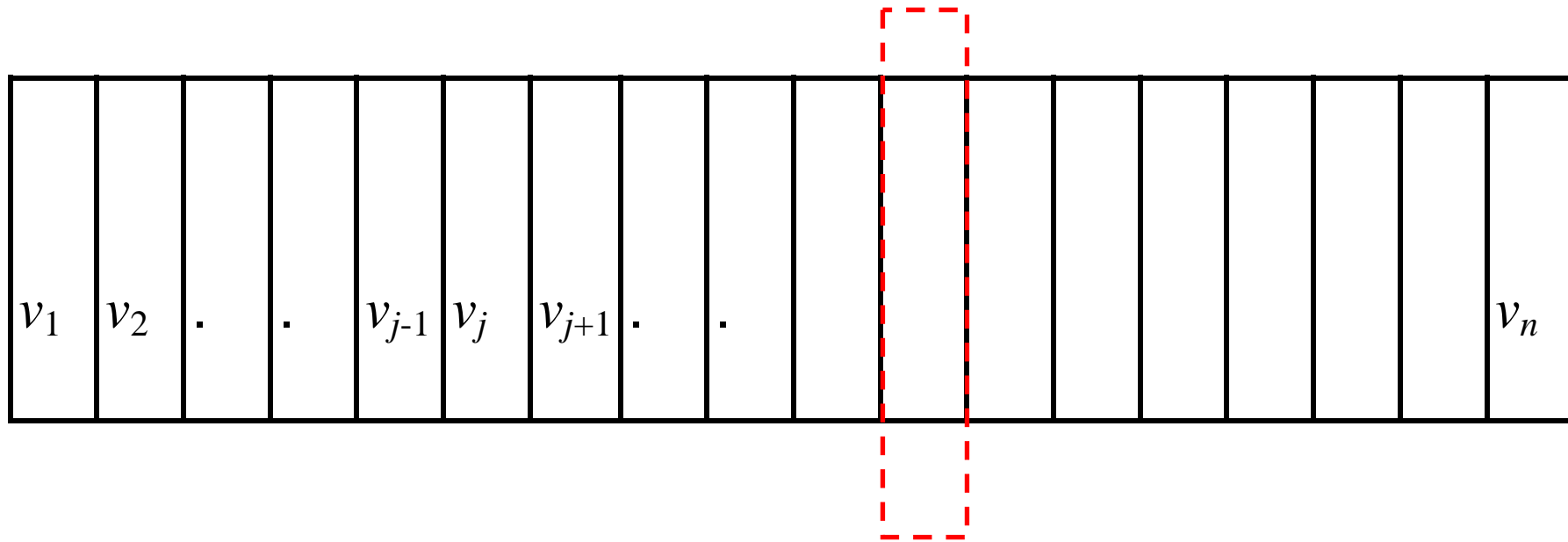
(Williams, 1986; Williams et al., 2006)

⇒ Randomization protection when spatial component not needed

⇒ Limits model selection mainly to component for small-scale spatial trends

⇒ Relatively easy to implement by small breeding companies

2. Nearest neighbour analysis (NNA)



v_j = Yield on j -th plot

A plot

Here: For simplicity, look at trend within a single array of plots (block)



Picture: Martin Zahner, Ihinger Hof

Differencing and Papadakis

First differences: $v_j - v_{j+1}$

Second difference: $v_j - \frac{v_{j-1} + v_{j+1}}{2}$

Papadakis: $v_j - b \frac{v_{j-1} + v_{j+1}}{2}$

(b is a regression parameter)

Second differences

$$z_j = v_j - \frac{v_{j-1} + v_{j+1}}{2}$$

Compute means per genotype:

$$y_i = \frac{\sum_{j \in S_i} z_j}{n_i}$$

S_i = set of plots with i -th genotype on internal plot

Linear model for second differences

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$$

where

$$\mathbf{y} = (y_1, y_2, \dots, y_s)'$$

$$\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_s)'$$

β_i = effect of the i -th cultivar ($i = 1, \dots, s$)

\mathbf{X} = is the corresponding design matrix; $\text{rank}(\mathbf{X}) = s-1, \mathbf{X}\mathbf{1} = \mathbf{0}$

\mathbf{e} = vector of independent and homoscedastic errors

Least squares estimation

$$\hat{\beta}_X = (X'X)^{-1} X'y \quad (\text{Wilkinson et al., 1983})$$

Estimates of cultivar means μ_i :

$$\hat{\mu}_i = \hat{\beta}_i - \bar{\hat{\beta}}_{\cdot} + \bar{v}_{\cdot}$$

Table 1: Toy yields of five cultivars tested in 10 plots arranged in two blocks of five plots.

Block	Cultivar i	Yield v_j	Second differences z_j
1	1	27	-3.0
1	3	33	6.0
1	5	27	-5.0
1	2	31	-5.5
1	4	46	17.0
2	1	34	-2.5
2	2	37	2.0
2	3	36	-8.5
2	4	52	16.0
2	5	36	-8.0
Mean:		35.9	

Table 2: Non-iterative least squares solution for toy data of Table 1 for second differences. Analysis based on cultivar means of second differences (y_i).

Cultivar	Design matrix X					ξ Estimates		
	i	1	2	3	4	5	y_i	$\hat{\beta}_i$
1	1	-0.25	-0.5	0	-0.25	-2.75	-0.50	30.65
2	-0.25	1	-0.25	-0.25	-0.25	-1.75	3.07	34.22
3	-0.25	-0.25	1	-0.25	-0.25	-1.25	3.38	34.52
4	0	-0.25	-0.25	1	-0.5	16.50	17.81	48.95
5	0	-0.25	-0.5	-0.25	1	-6.50	0.000	31.14
Mean:								35.90

The algorithm of Schwarzbach (1984)

- (i) Initialize estimates of the cultivar effects β_i ($i = 1, \dots, s$). Set $k = 0$.
- (ii) For every plot in a column (block) compute second differences z_j .
For each cultivar, compute the mean

$$y_i = \frac{\sum_{j \in S_i} z_j}{n_i} .$$

- (iii) Compute $\Delta_k = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}_k$ and update the current estimates by
 $\boldsymbol{\beta}_k \leftarrow \boldsymbol{\beta}_k + \Delta_k$. When convergence of $\Delta_k^T \Delta_k$ has been achieved, stop.
Else set $k \leftarrow k + 1$ and repeat (iii).
- (iv) At convergence (iteration m) the solution is centered by
 $\boldsymbol{\beta}_m \leftarrow (\mathbf{I} - a^{-1}\mathbf{J})\boldsymbol{\beta}_m$ and mean estimates are computed by $\mathbf{1}\bar{v}_{\bullet} + \boldsymbol{\beta}_m$.

Software

- ANOFT (written by Erik Schwarzbach, Czech Republic)
- AGROBASE (Agromix Software Inc., Canada)

Both packages are widely used by plant breeding companies

Properties of Schwarzbach's algorithm

Defining $A = (I - X)$ and $M_m = \sum_{k=0}^{m-1} A^k$, Schwarzbach's estimator takes form

$$\beta_m = M_m y + A^m \beta_0,$$

Theorem 1: Equation (1) converges to a solution for β in the consistent

equation $\tilde{X}\tilde{\beta} = y$, where $\tilde{X} = (\mathbf{1} \quad X)$ and $\tilde{\beta} = (\theta, \beta^T)^T$.

(Proof: [Piepho, Richter and Williams, 2008, *Biometrical Journal*](#))

⇒ Schwarzbach's algorithm fits an intercept to first differences!

Table 3: Non-iterative least squares solution for toy data based on cultivar means of second differences (y_i).

Cultivar		Without intercept		With intercept [§]	
i	y_i	$\hat{\beta}_i$	$\hat{\mu}_i$	$\hat{\beta}_i$	$\hat{\mu}_i$
1	-2.75	-0.50	30.65	-0.68	30.54
2	-1.75	3.07	34.22	2.99	34.20
3	-1.25	3.38	34.52	3.39	34.60
4	16.50	17.81	48.95	17.72	48.94
5	-6.50	0.000	31.14	0.00	31.22
Mean:			35.90	35.90	

§ $\hat{\theta} = 0.37$. Solution for means equal to that by Schwarzbach's method.

An improvement

n_i may not be constant \Rightarrow

Fit model directly to observed differences z_j (not $y_i = \text{cultivar means of } z_i$):

$$\mathbf{z} = \mathbf{W}\boldsymbol{\beta} + \mathbf{f},$$

where

$$\mathbf{z} = (z_1, z_2, \dots)'$$

$$\hat{\boldsymbol{\beta}}_W = (\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}'\mathbf{z} \neq \hat{\boldsymbol{\beta}}_X$$

First differences

Compared to second differences, a milder adjustment for trend is

$$r_j = v_j - v_{j+1}$$

Analysis assumes that r_j are independent normal deviates.

Relation to second differences:

$$z_j = \frac{r_j - r_{j-1}}{2} = \frac{v_j - v_{j+1} - (v_{j-1} - v_j)}{2} = v_j - \frac{v_{j-1} + v_{j+1}}{2}$$

If at border plots $z_j = r_j/2$, then OLSE based on y_i and r_j are equivalent!

(Besag and Kempton, 1986)

[Problem: Measurement error associated with yields v_j is ignored.]

3. Linear variance structures

Basic trend model:

$$v_j = \theta + \beta_{(j)} + t_j$$

θ = constant

$\beta_{(j)}$ = effect of treatment on plot j

t_j = spatial trend on j -th plot

Random walk

Trend component:

$$t_{j+1} = t_j + a_{j+1}$$

t_j = fertility trend associated with v_j

$$a_j \sim N(0, \sigma_a^2)$$

Starting level t_0 : fit a fixed effect

Fit random walk using mixed model package

$$\text{var}(\mathbf{t}) = \text{var}(t_1, t_2, \dots) = \mathbf{A}_n \sigma_a^2$$

$$\mathbf{A}_n = \{\min(i, j)\} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & . & 1 \\ 1 & 2 & 2 & 2 & 2 & . & . \\ 1 & 2 & 3 & 3 & 3 & . & . \\ 1 & 2 & 3 & 4 & 4 & . & . \\ 1 & 2 & 3 & 4 & . & . & . \\ . & . & . & . & . & . & n-1 \\ 1 & . & . & . & . & n-1 & n \end{pmatrix}$$

SAS PROC MIXED \Rightarrow TYPE=LIN(1)

(Piepho and Ogutu, 2007)

A problem

Walking direction and placement of origin (t_0) not unique

\Rightarrow Choice of A_n not unique

Solution: fit fixed effect $t_0 =$ fixed block effect

$\Leftrightarrow (I_n - K_n)A_n(I_n - K_n)$ unique, where $K_n = n^{-1}\mathbf{1}\mathbf{1}'$

Model for first differences

$$r_j = v_j - v_{j+1} = \beta_{(j)} - \beta_{(j+1)} - a_{j+1}$$

$$a_j \sim N(0, \sigma_a^2)$$

Log-likelihoods for original data under random walk and for first differences:

$$\log L = -\frac{1}{2}(n-1)\log(2\pi\sigma_a^2) - \frac{1}{2\sigma_a^2} \sum_{j=1}^{n-1} (v_j - v_{j+1} - \beta_{(j)} + \beta_{(j+1)})^2$$

Restricted log-likelihoods are also identical

Linear variance (LV) model (Williams, 1986)

$$\text{var}(\mathbf{t}) = \text{var}(t_1, t_2, \dots) = \mathbf{V} = \eta \mathbf{J}_n - \phi \mathbf{L}_n$$

$$\mathbf{L}_n = \{|j_1 - j_2|\} = \begin{pmatrix} 0 & 1 & 2 & 3 & \dots & n-1 \\ 1 & 0 & 1 & 2 & \dots & n-2 \\ 2 & 1 & 0 & 1 & \dots & \dots \\ 3 & \dots & 1 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & 2 \\ \dots & \dots & \dots & \dots & 0 & 1 \\ n-1 & \dots & \dots & 2 & 1 & 0 \end{pmatrix}$$

$$\text{var}(v_{j_1} - v_{j_2}) = 2\phi |j_1 - j_2| \hat{=} \text{first differences} \hat{=} \text{random walk}$$

Table 4: Estimates of cultivar effects and means for toy data in Table 1 based on three different analyses.

Cultivar	Second differences (z_j)		First differences (r_j)		Original data (v_j) (Linear variance)	
	$\hat{\beta}_i$	§ $\hat{\mu}_i$	$\hat{\beta}_i$	§ $\hat{\mu}_i$	$\hat{\beta}_i$	$\hat{\mu}_i$
1	-0.68	30.39	-0.63	30.20	-0.63	30.50
2	3.49	34.56	3.68	34.50	3.68	34.80
3	3.44	34.52	4.08	34.90	4.08	35.20
4	17.89	48.96	18.25	49.08	18.25	49.38
5	0	31.07	0	30.83	0	31.13
Mean:		35.90		35.90		36.20

§ Means computed as $\hat{\mu}_i = \hat{\beta}_i - \overline{\hat{\beta}}_{\bullet} + \bar{v}_{\bullet}$.

Errors in variables (nugget effect)

$$v_j = \theta + \beta_{(j)} + t_j + e_j$$

$\beta_{(j)}$ = effect of treatment on plot j

t_j = spatial trend on j -th plot

e_j = measurement error on j -th plot; $e_j \sim N(0, \sigma^2)$

$$\text{var}(\mathbf{v}) = \text{var}(v_1, v_2, \dots) = \mathbf{V} = \mathbf{J}_n \boldsymbol{\eta} - \mathbf{L}_n \boldsymbol{\phi} + \mathbf{I}_n \sigma^2$$

Pairwise variance:

$$\text{var}(v_{j_1} - v_{j_2}) = 2[\sigma^2 + |j_1 - j_2| \phi]$$

A reparameterization to ensure $V > 0$

Require $\eta \mathbf{J}_n - \phi \mathbf{L}_n > 0$.

\Rightarrow Reparameterize as $\eta' \mathbf{J}_n + \phi \mathbf{M}_n$, where

$$\mathbf{M}_n = (n-1)\mathbf{J}_n - \mathbf{L}_n \quad \text{and} \quad \eta' = \eta - (n-1)\phi \quad \text{and}$$

require $\eta', \phi \geq 0$

$$\Rightarrow V = \sigma^2 \mathbf{I}_n + \eta' \mathbf{J}_n + \phi \mathbf{M}_n.$$

Interpretation of LV model

$$V = V_0 + V_S ,$$

where

$$V_0 = \sigma^2 I_n + \tilde{\eta} J_n \quad (\text{Classical block model})$$

$$V_S = \kappa (J_n + \tilde{\phi} M_n), \quad (\text{Spatial add-on})$$

with $\tilde{\eta} = \eta' - \kappa$ and $\tilde{\phi} = \kappa^{-1} \phi$

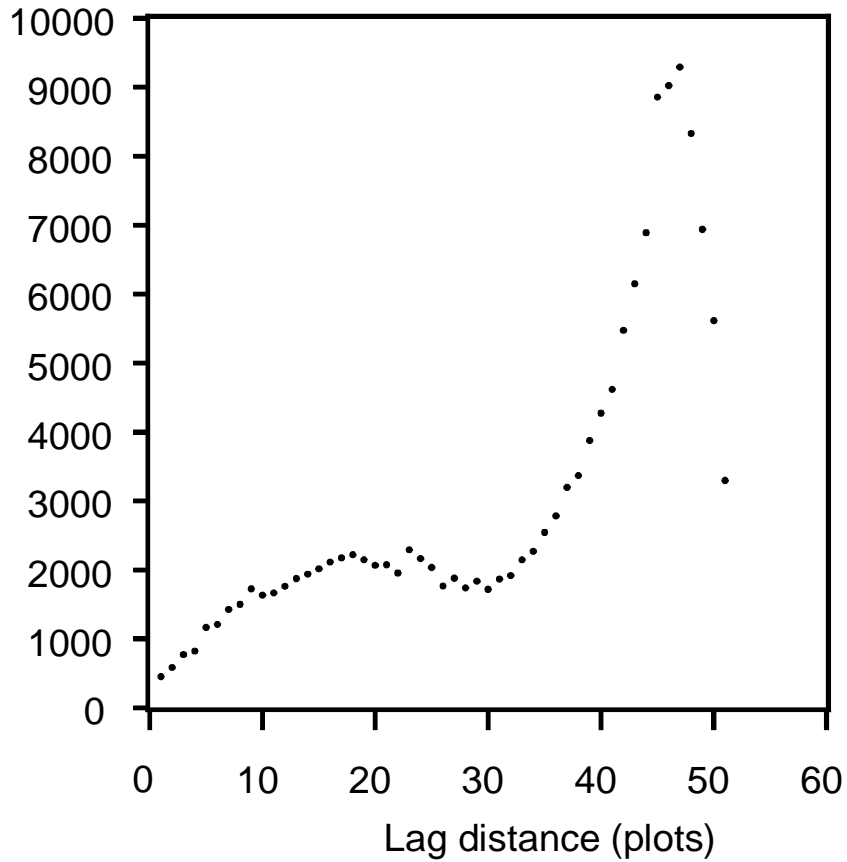
Interpretation of LV model

(i) $\sigma^2 \mathbf{I}_n$ in V_0 models plot and measurement error (nugget effect or white noise in geostatistical parlance)

(ii) $\tilde{\eta} \mathbf{J}_n$ in V_0 models block effects as arising from randomization theory. In a more geostatistically motivated view, the block effects capture “extraneous variation” due to technical causes such as tractor reeling etc. (Gilmour et al. 1997)

(iii) V_s models a spatial correlation within a block by a linear variance-covariance structure where correlation decays linearly with distance (Williams 1986)

(a) Robust semi-variogram for observed data



(b) Robust semi-variogram for first differences

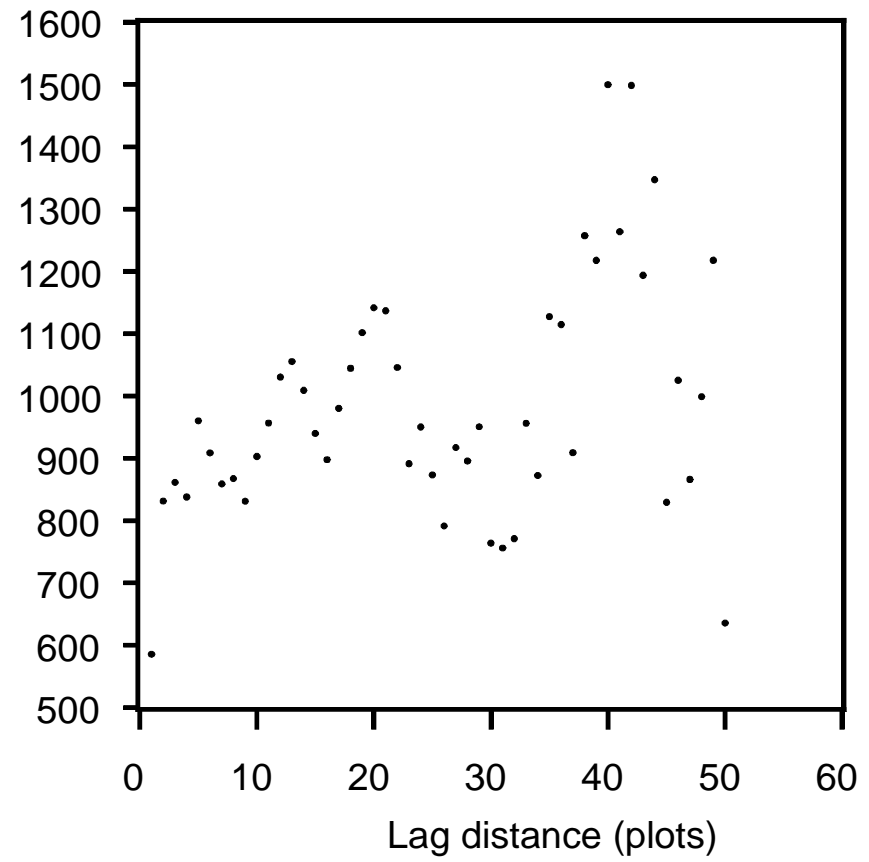


Fig. 1: Variograms for wheat data in Besag and Kempton (1986).
[52 x 7 grid of plots, 2 varieties grown in chessboard pattern]

Table: Restricted maximum likelihood (REML) fits for wheat data of Besag and Kempton (1986). Columns subdivided into 8 blocks alternating in size between 6 and 7.

Variance-covariance model	$-2 \log L_R$	s.e. $(\hat{\beta}_1 - \hat{\beta}_2)$	$\hat{\rho}$
Fixed blocks (7 columns, 8 blocks each):			
Nugget only (baseline)	2983.4	2.7521	-
Random walk	2993.2	1.7890	-
Linear variance	2993.2	1.7890	-
AR(1)	2955.1	2.0827	0.4020
Random walk + nugget	2951.3	2.2417	-
Linear variance + nugget	2951.3	2.2417	-
AR(1) + nugget	2950.8	2.2089	0.8697
Random blocks (7 columns, 8 blocks each):			
Linear variance	3553.5	1.7684	-
AR(1)	3514.7	2.0697	0.4122
Linear variance + nugget	3508.5	2.2248	-
AR(1) ⁺ + nugget	3508.6	2.2044	0.9069

LV approximates AR(1)

LV model: $V_S = \kappa \{1 - \tilde{\phi} |j_1 - j_2|\}$

AR(1) model: $V_S = \kappa \{\rho^{|j_1 - j_2|}\}$

$$\rho \approx 1 \Rightarrow \rho^{|j_1 - j_2|} \approx 1 - \tilde{\phi} |j_1 - j_2| \text{ with } \tilde{\phi} = -\log(\rho)$$

4. Nugget-variogram

$$\mathbf{v} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \mathbf{e}$$

$$\begin{aligned} \mathbf{e} &= \text{nugget effect} \quad ; & \mathbf{e} &\sim \text{MVN}(\mathbf{0}, \sigma^2 \mathbf{I}) \\ \mathbf{u} &= \text{all other random effects} \quad ; & \mathbf{u} &\sim \text{MVN}(\mathbf{0}, \mathbf{G}) \end{aligned}$$

Semivariance:

$$s_{ij} = \frac{1}{2}(e_i - e_j)^2$$

Plot $E(s_{ij})$ versus distance of plots i and j along rows and columns

\Rightarrow expect horizontal plane when model is adequate: $E(s_{ij}) = \sigma^2$

Bias correction variogram (Gilmour et al. 1997)

$$\hat{e} = y - (X\hat{\beta} + Z\hat{u})$$

$$\hat{e} \sim N(\mathbf{0}, R - W'C^{-1}W) , \text{ where}$$

$$W = [X \quad Z] \text{ and } C = \text{coefficient matrix of mixed model equations}$$

Estimated semivariance:

$$E(\hat{s}_{ij}) = \frac{1}{2}(\hat{e}_i - \hat{e}_j)^2 = s_{ij} - \frac{1}{2}\mathbf{a}'_{ij}W'C^{-1}W\mathbf{a}_{ij}$$

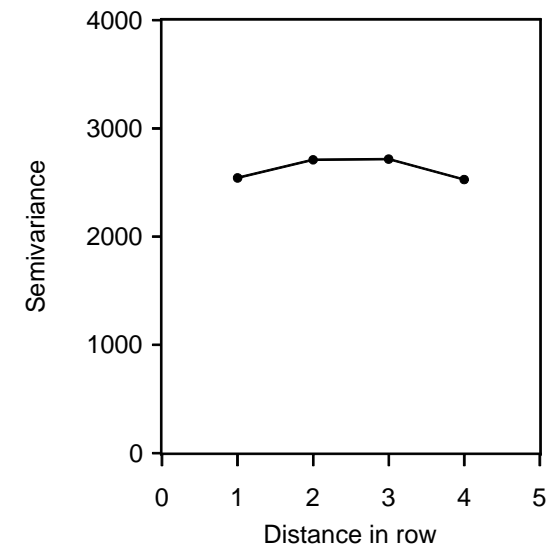
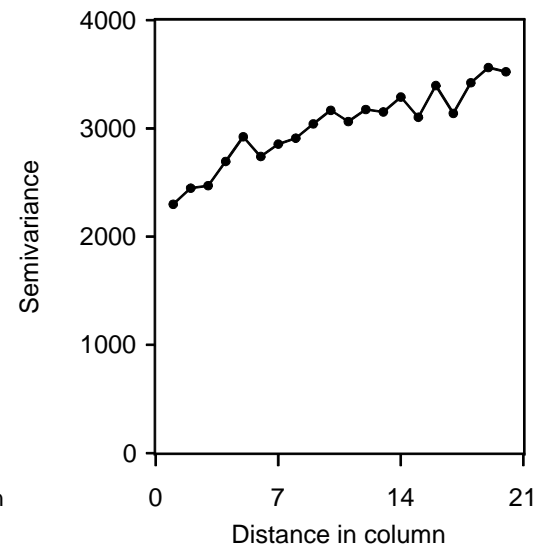
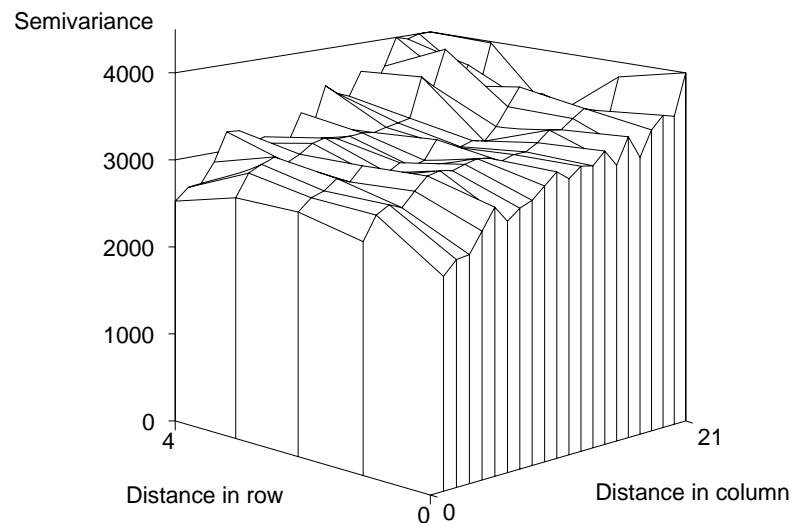
\mathbf{a}_{ij} = vector of zeros except 1 for obs. i and -1 for obs. j

5. Examples from field experiments

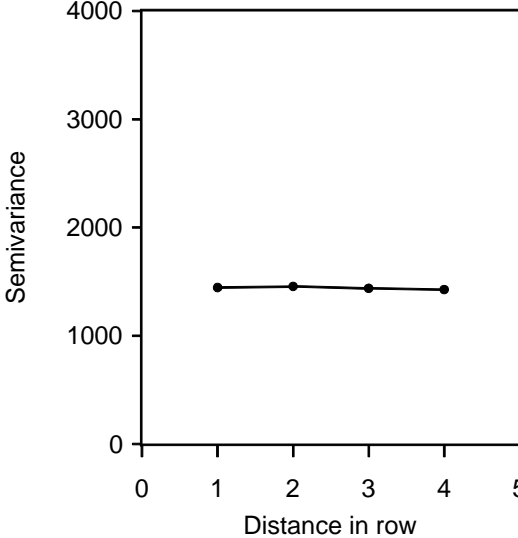
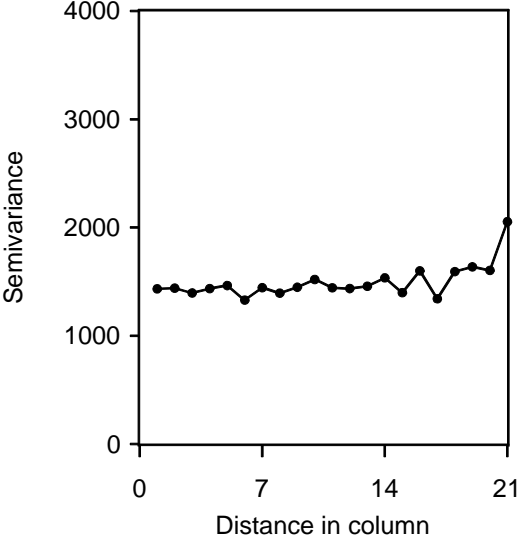
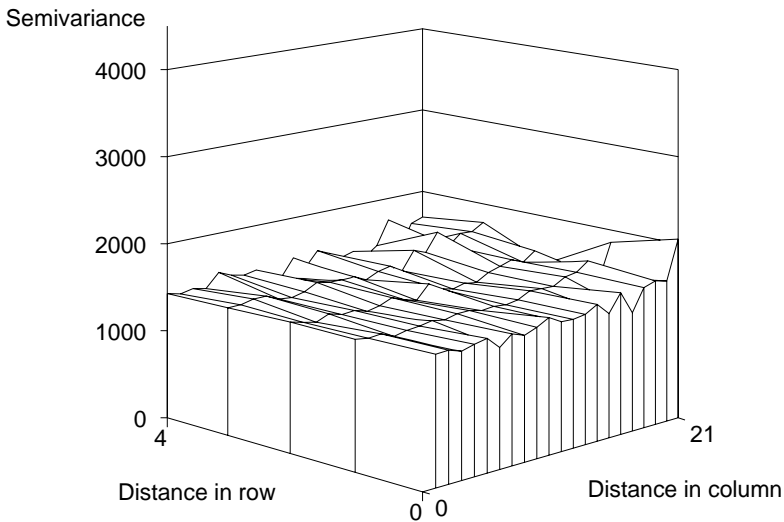
Example 1: Wheat data (from Gilmour et al., 1997)

- 104 varieties
- Randomized block design with 3 blocks (22 columns, 5 rows)
- Some varieties had two plots in a block

Baseline model

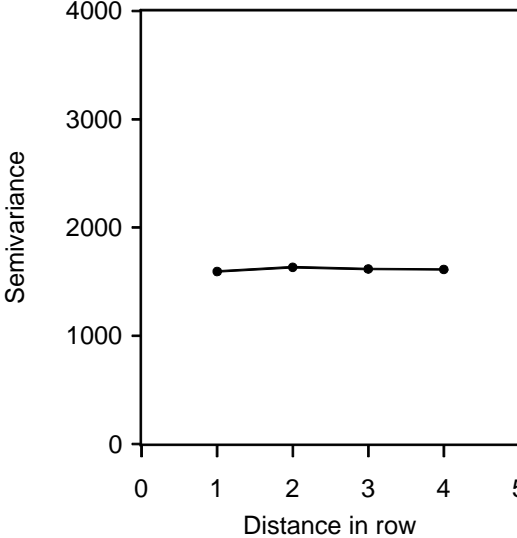
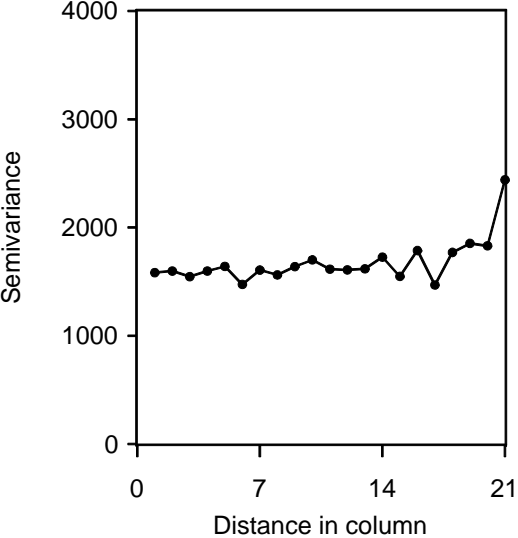
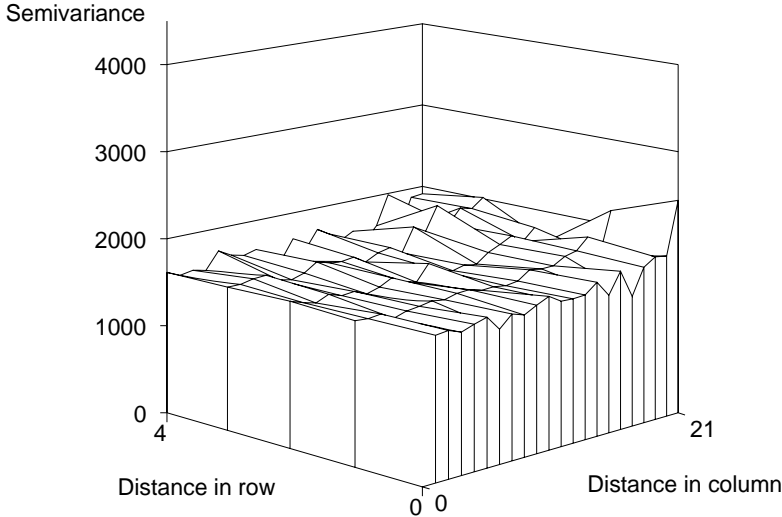


Baseline + Linear variance (LV) in columns



Drop in deviance (REML) compared to baseline = 32.0

Baseline + LV+LV

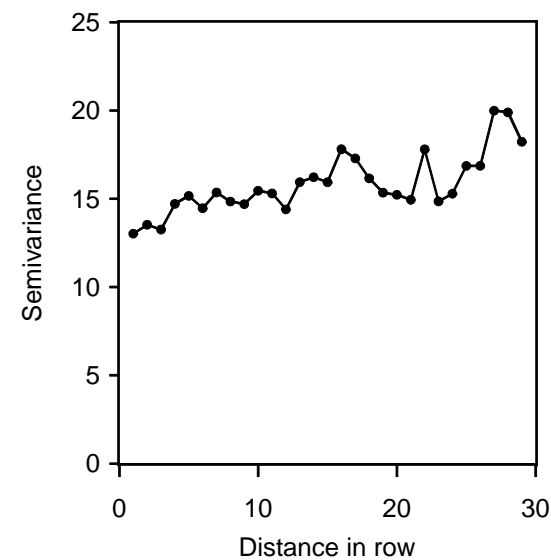
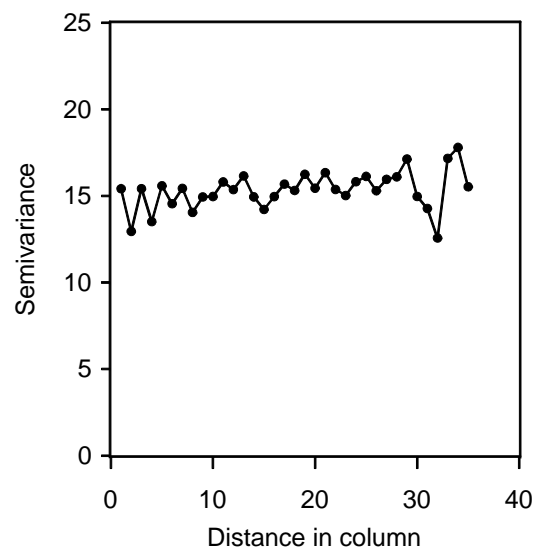
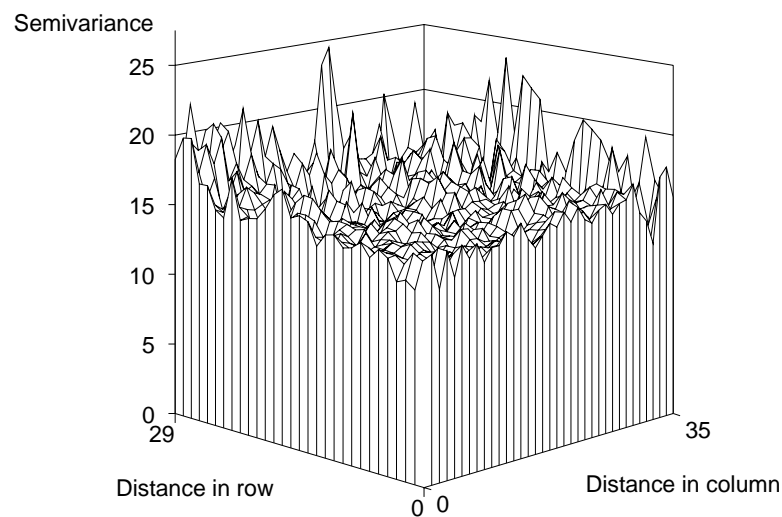


Drop in deviance compared to LV in columns = 0.3

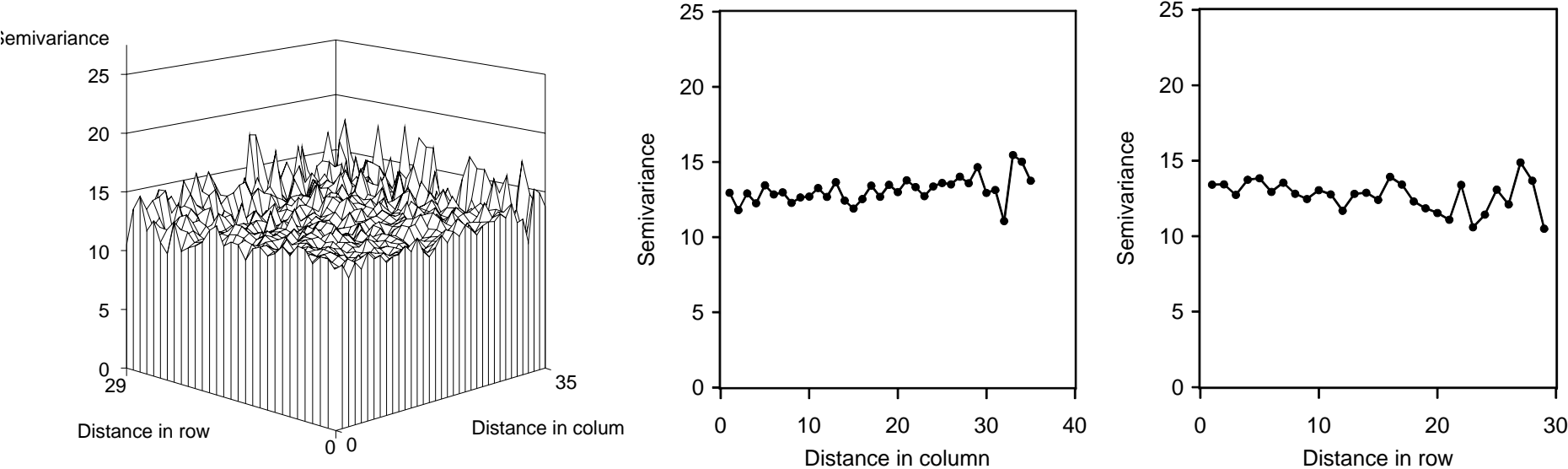
Example 2: Uniformity trial (spring barley)

- 36 x 30 plots
- Plot widths: 1.90 m along rows and 3.73 m along columns

Baseline model

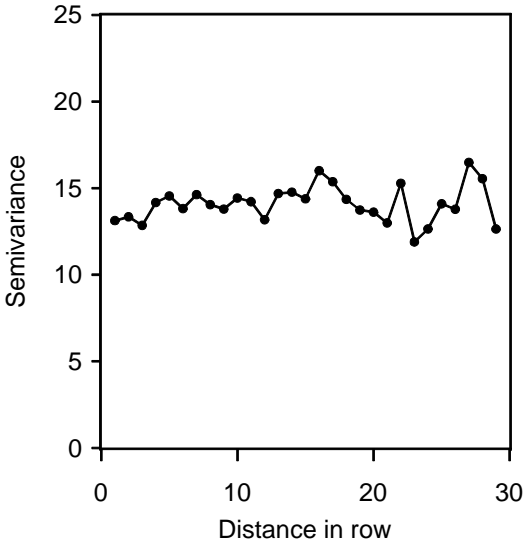
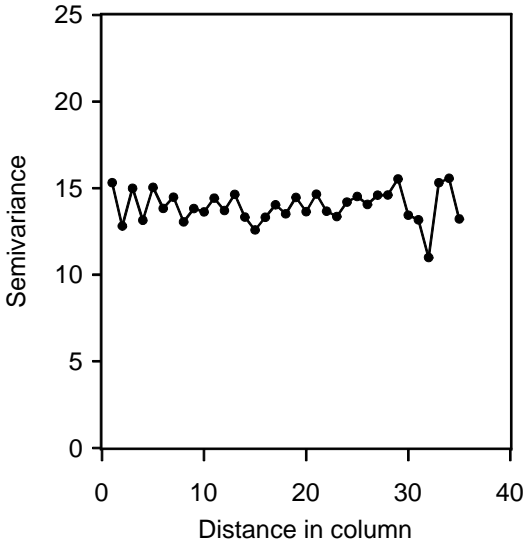
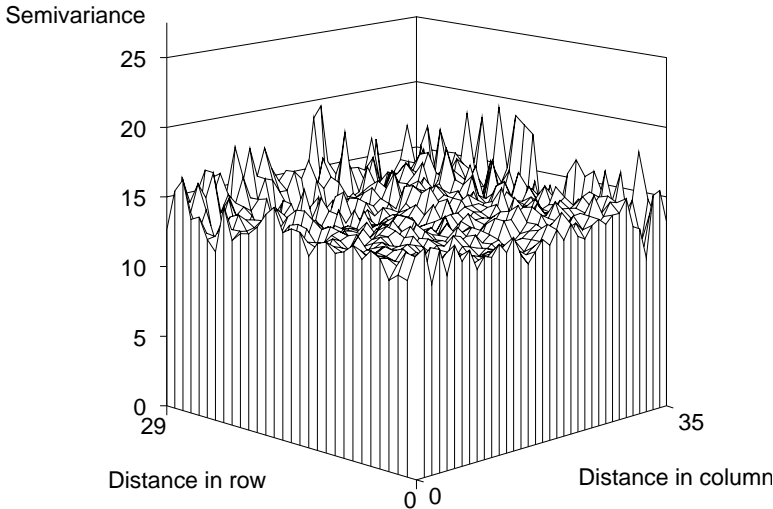


Baseline + Linear variance in columns (LV⊗I)



Drop in deviance (REML) compared to baseline = 52.4

Baseline + LV⊗LV



Drop in deviance compared to LV in columns = 26.1

Table 5: Deviances and values of the Akaike Information Criterion (AIC) for uniformity trial with spring barley.

Model	Deviance	AIC
Baseline (row+column+nugget)	6114.8	6120.8
Baseline + AR(1) \otimes I ^[1]	6068.7	6076.7
Baseline + AR(1) \otimes AR(1) ^[2]	6042.7	6054.7
Baseline + LV \otimes I	6067.2	6077.2
Baseline + LV+LV	6056.3	6070.3
Baseline + LV \otimes J	6107.8	6115.8
Baseline + LV \otimes LV [§]	6041.1	6051.1

§ ϕ'_R converged to zero.

[1] $\rho_C=0.9308$

[2] $\rho_R= 0.9705$; $\rho_C = 0.9671$

Example 3: 174 sugar beet trials

- Sugar beet breeding trials by KWS SAAT AG Einbeck, Germany
- Testcrosses (hybrids) of doubled-haploid (DH) lines
- Years 2003 to 2005
- Six locations
- Up to 10 trials per location and year
- Each trial laid out as a 10x10 lattice design
- Five blocks of size 10 formed a column
- Two columns formed a replicate
- Two or three replicates
- Plots were 7.5 m wide along rows and 1.5 m wide down the columns
⇒ main trend expected down columns

Table 6: Number of times a model type was selected for the sugar beet trials using AIC. Spatial models allow spatial covariance to extend across whole trial.

	2003	2004	2005
Baseline (row+column+nugget)	1	3	5
Baseline + $I \otimes AR(1)$	7	6	5
Baseline + $AR(1) \otimes AR(1)$	24	6	7
Baseline + $I \otimes LV$	4	11	8
Baseline + $LV+LV$	4	8	14
Baseline + $J \otimes LV$	0	8	4
Baseline + $LV \otimes LV$	20	18	11

Table 7: Median of autocorrelation estimates for sugar beet trials. Spatial models allow spatial covariance to extend across whole trial.

Median ρ_R	0.94	0.94	0.91
Median ρ_C	0.57	0.36	0.36
Median % nugget [§]	25	47	37
Total number of trials	60	60	54

§ Ratio of nugget variance over sum of nugget and spatial variance.

Table 8: Number of times a model type was selected for the sugar beet trials using AIC, and median of autocorrelation estimates. Spatial covariance modelled within blocks of 10 x 10 lattice design only.

	2003	2004	2005
Selected model type:			
Baseline (repl+block+nugget)	17	38	29
Baseline + AR(1) in blocks	7	2	3
Baseline + LV in blocks	36	20	22
Median of parameter estimates for AR(1) model:			
Median ρ	0.93	0.93	0.81
Median % nugget [§]	36	54	53
Total number of trials	60	60	54

§ Ratio of nugget variance over sum of nugget and spatial variance.

6. Summary

- Model observed data (linear variance) rather than differences
- Use efficient block or row-column design
- Use randomization-based mixed model as baseline for analysis
- Explore spatial as an add-on within replicates or blocks only
- Use likelihood and variograms for model selection
- First check for main direction of trend; then check if two-dimensional extension is needed
- Can numerically search optimal spatial design

Own literature

Lee, Y., Piepho, H.P. (2008). Ambiguity in random walks and implications for the analysis of one- or two-dimensional spatial or time-structured data.
(submitted).

Piepho, H.P., Ogutu, J.O. (2007). Simple state-space models in a mixed model framework. *The American Statistician* **61**, 224-232.

Piepho, H.P., Richter, C., Williams, E.R. (2008). On the use of nearest neighbour adjustment and linear variance models in plant breeding trials.
Biometrical Journal **50**, 164-189.

Piepho, H.P., Williams, E.R. (2008). Linear variance structures for field trials
(submitted).

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4. Extensions of the linear variance model in two dimensions

Columns

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Rows

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General form of model

$$\text{var}(v) = I_r \otimes V = I_r \otimes (V_0 + V_S) ,$$

r replicates

s columns within replicates

k rows within replicates

V_S = spatial structure

V_0 = baseline model

Baseline model

$$V_0 = \sigma^2 \mathbf{I}_s \otimes \mathbf{I}_k + \eta_C \mathbf{I}_s \otimes \mathbf{J}_k + \eta_R \mathbf{J}_s \otimes \mathbf{I}_k$$

s = no. of columns; k = no. of rows

σ^2 = nugget variance

η_C and η_R = variance for columns and rows, respectively

Interpretation

- (i) **randomization** according to a resolvable (spatial) row-column design
- (ii) presence of **extraneous variation**

Spatial add-on component (LV+LV):

Super-imposed row structure:

$$\mathbf{I}_s \otimes (\eta_C \mathbf{J}_k + \phi_C \mathbf{M}_k)$$

Super-imposed column structure:

$$(\eta_R \mathbf{J}_s + \phi_R \mathbf{M}_s) \otimes \mathbf{I}_k$$

Add to have more flexibility:

$$\phi_{RC} \mathbf{M}_{sk}$$

$$\mathbf{M}_{sk} = (s-1)(k-1) \mathbf{J}_s \otimes \mathbf{J}_k - \mathbf{L}_s \otimes \mathbf{L}_k$$

$$\Rightarrow \mathbf{V}_S = \phi_C \mathbf{I}_s \otimes \mathbf{M}_k + \phi_R \mathbf{M}_s \otimes \mathbf{I}_k + \phi_{RC} \mathbf{M}_{sk}$$

with constraints $\phi_R, \phi_C, \phi_{RC} > 0$

(Williams et al., 2006)

Spatial add-on component ($LV \otimes LV$):

$$V_S = \kappa V_R \otimes V_C \quad (\text{a separable structure})$$

where

$$V_R = \mathbf{J}_s - \phi_R \mathbf{L}_s \quad \text{and} \quad V_C = \mathbf{J}_k - \phi_C \mathbf{L}_k$$

Correlation of two plots (i_1, j_1) and (i_2, j_2) : $(1 - \phi_R |j_1 - j_2|)(1 - \phi_C |i_1 - i_2|)$,

$$\kappa^{-1} V_S = \mathbf{J}_s \otimes \mathbf{J}_k - \phi_C \mathbf{J}_s \otimes \mathbf{L}_k - \phi_R \mathbf{L}_s \otimes \mathbf{J}_k + \phi_R \phi_C \mathbf{L}_s \otimes \mathbf{L}_k$$

(Piepho and Williams, 2008)

Reparameterization to ensure that $V > \mathbf{0}$

$$V_R = \lambda_R \mathbf{J}_s + \phi_R \mathbf{M}_s \quad \text{and} \quad V_C = \lambda_C \mathbf{J}_k + \phi_C \mathbf{M}_k, \quad \text{where}$$

$$\lambda_R = 1 - (s-1)\phi_R \quad \text{and} \quad \lambda_C = 1 - (k-1)\phi_C \quad \text{with} \quad 0 \leq \lambda_R, \lambda_C \leq 1,$$

whence

$$K^{-1}V_S = \lambda_R \lambda_C \mathbf{J}_s \otimes \mathbf{J}_k + \lambda_R \phi_C \mathbf{J}_s \otimes \mathbf{M}_k + \phi_R \lambda_C \mathbf{M}_s \otimes \mathbf{J}_k + \phi_R \phi_C \mathbf{M}_s \otimes \mathbf{M}_k$$

Reparameterize $LV \otimes LV$ model as a linear structure

Can drop $\lambda_R \lambda_C \mathbf{J}_s \otimes \mathbf{J}_k$ because it is confounded with fixed replicate effect

$$V_S = \phi'_C \mathbf{J}_s \otimes \mathbf{M}_k + \phi'_R \mathbf{M}_s \otimes \mathbf{J}_k + \phi'_{RC} \mathbf{M}_s \otimes \mathbf{M}_k$$

where

$$\phi'_C = \kappa \lambda_R \phi_C \geq 0, \quad \phi'_R = \kappa \lambda_C \phi_R \geq 0, \quad \phi'_{RC} = \kappa \phi_C \phi_R \geq 0$$

For comparison: separable AR(1) model

$$V_S = K V_R \otimes V_C \quad (\text{a separable structure})$$

where

$$V_R = \left\{ \rho_R^{|i_1 - i_2|} \right\}$$

$$V_C = \left\{ \rho_C^{|j_1 - j_2|} \right\}$$

Spatial design

Fit fixed row and column effects, i.e., sweep out row and column effects:

$$\boldsymbol{w} = \boldsymbol{S}_{RC} \boldsymbol{v}$$

$$\boldsymbol{S}_{RC} = \boldsymbol{I}_r \otimes (\boldsymbol{I}_s - \boldsymbol{K}_s) \otimes (\boldsymbol{I}_k - \boldsymbol{K}_k) \quad , \quad \text{where} \quad \boldsymbol{K}_k = k^{-1} \boldsymbol{J}_k \quad ,$$

$$\Rightarrow \text{var}(\boldsymbol{w}) = \boldsymbol{S}_{RC} \boldsymbol{V} \boldsymbol{S}_{RC}$$

LV+LV: $\text{var}(\boldsymbol{w})$ depends on ϕ_R , ϕ_C , ϕ_{RC} and σ^2

LV \otimes LV: $\text{var}(\boldsymbol{w})$ depends on ϕ'_{RC} and σ^2 only

Intrarow and intracolumn information matrix for LV+LV: (Williams et al., 2006)

$$A = rI_t - X'(I_r \otimes W_R \otimes W_C)X, \text{ where}$$

$$W_C = -(I_k - K_k)U_k(I_k - K_k) + K_k, \quad U_k = 3L_k/(k^2 - 1), \text{ and}$$

X = treatment design matrix

Spatial average efficiency factor:

$$E = \frac{t-1}{r \text{ trace}(A^+)}$$

⇒ Search algorithm in CycDesignN 3.0

LV⊗LV: It seems we can use the same efficiency factor (work in progress)!