Beyond RCBD

Design-Based Versus Model-Based Approaches to Account for Spatial Heterogeneity

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Gylling Data Management

Beyond RCBD

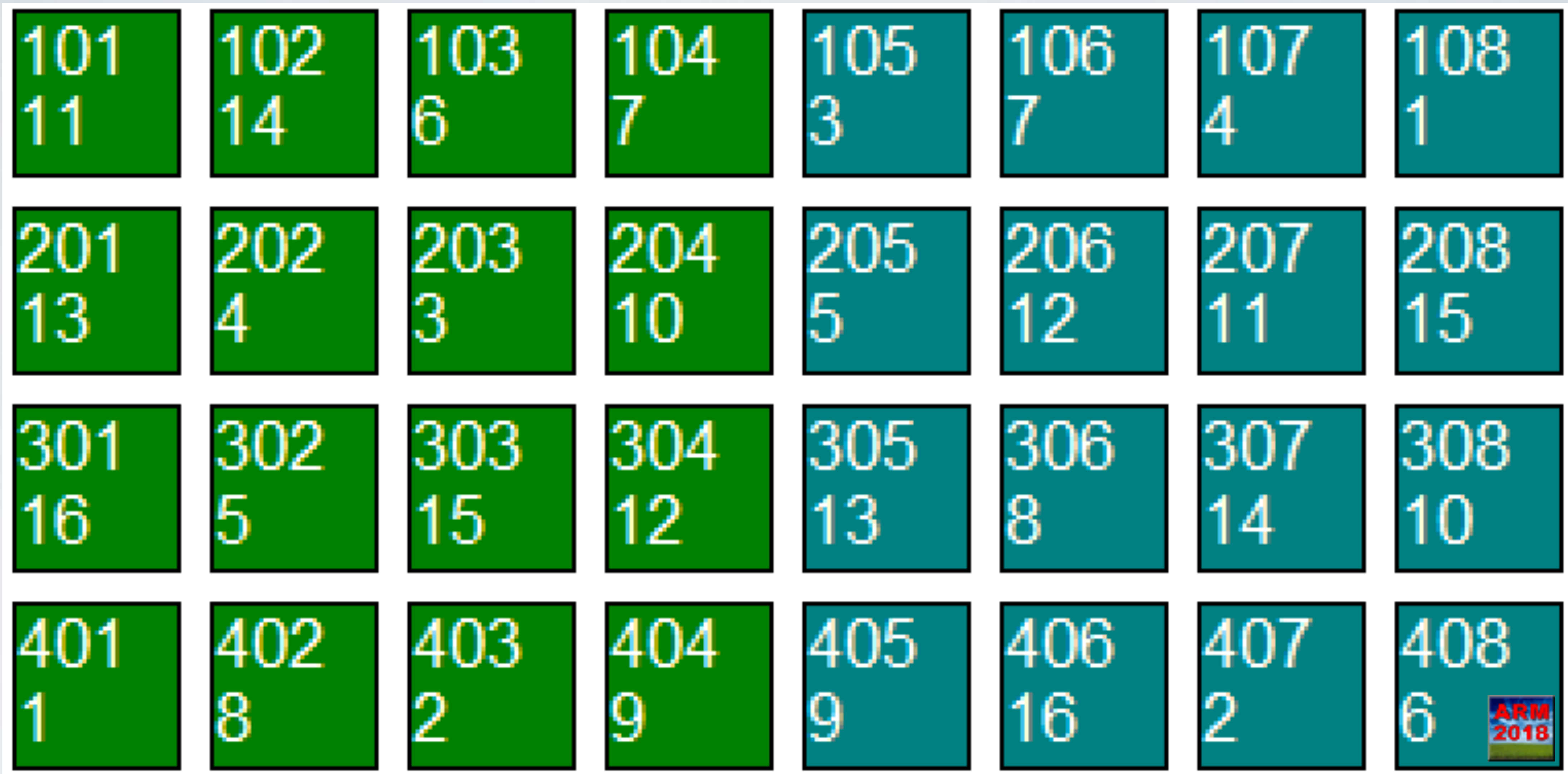
- Statistical models for analysis beyond the randomized complete block model.
- Experimental designs for blocking beyond the randomized complete block design.

A Motivating Example

- Cochran, W. G. (1947). Some consequences when the assumptions for the analysis of variance are not satisfied. Biometrics, 3(1), 22–38.
- *7. Effects of Correlations Amongst the Errors*

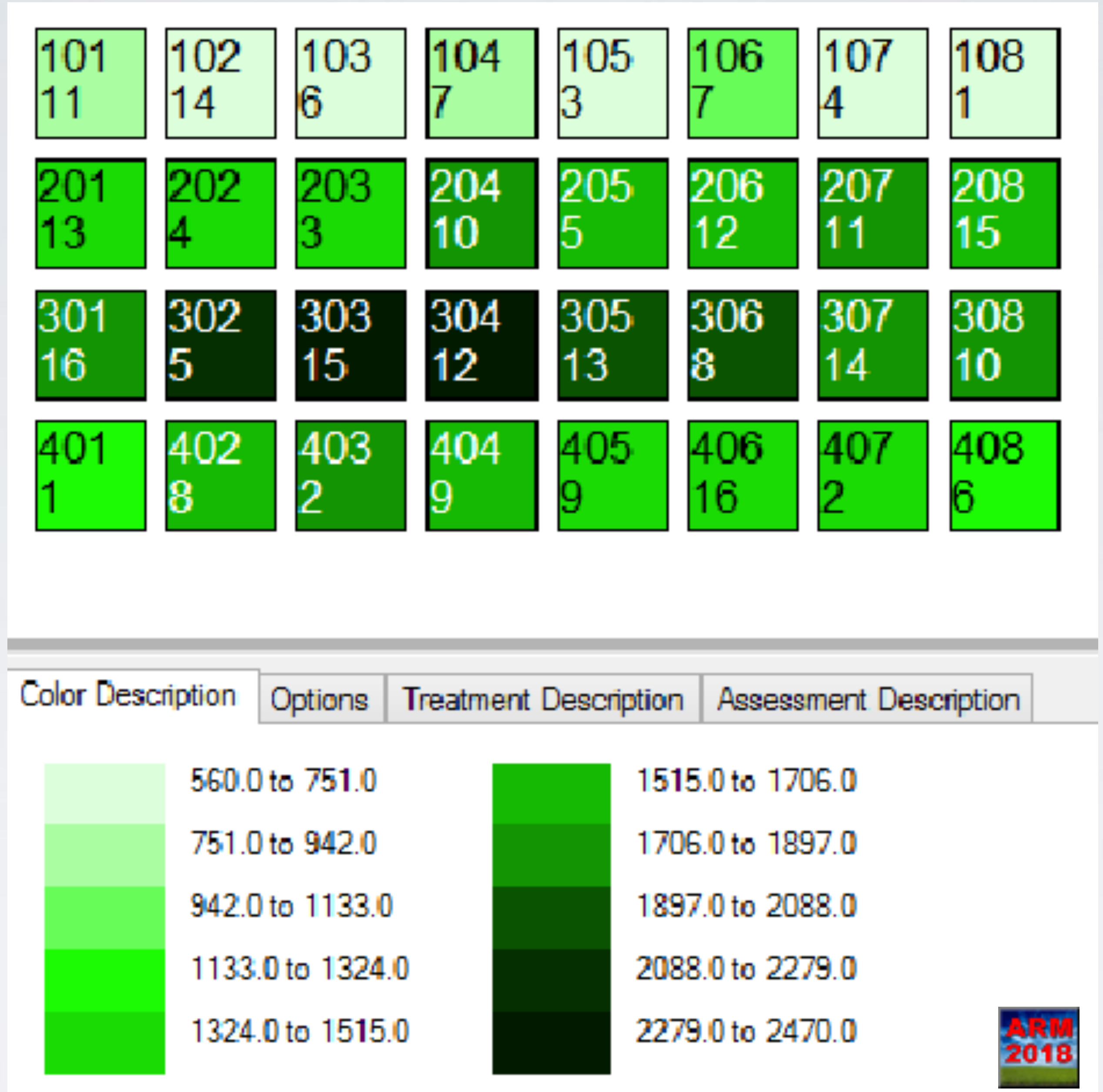
Cochran (1947)

- *Occasionally it may be discovered that the data have been subject to some systematic pattern of environmental variation that the randomization has been unable to cope with. If the environmental pattern obviously masks the treatment effect, resort may be had to what might be called desperate remedies in order to salvage some information.*



An Instance of Correlated Error

A 2^4 factorial experiment in two replicates (lime, fish manure, artificial fertilizers, one or two years application).



Yield Map

Values are plot yield (heads of pyrethrum, dry weight, gm)

Cochran (1947)

- *It is evident that the first row of plots is of poor fertility—treatments appearing in that row have only about half the yields that they give elsewhere. Further, there are indications that every row differs in fertility, the last row being second worst and the third row best. The fertility gradients are especially troublesome in that the four untreated controls all happen to lie in outside rows. The two replications give practically identical totals and remove none of the variation.*

101 11	102 14	103 6	104 7	105 3	106 7	107 4	108 1
201 13	202 4	203 3	204 10	205 5	206 12	207 11	208 15
301 16	302 5	303 15	304 12	305 13	306 8	307 14	308 10
401 1	402 8	403 2	404 9	405 9	406 16	407 2	408 6

Analysis of Variance

Randomized Complete Block (RCB) Least square estimation AOV For CHYCI Pyr

Source	DF	Sum of Squares	Mean Square	F	Prob(F)
Total	31	8046621.875000			
Replicate	1	65703.125000	65703.125000	0.291	0.5976
Treatment	15	4592071.875000	306138.125000	1.355	0.2818
Error	15	3388846.875000	225923.125000		

The replicates remove so little variation that we would get a better result analyzing the experiment as a completely random design.

Completely Random (Fully Randomized) Least square estimation AOV For CHYCI

Source	DF	Sum of Squares	Mean Square	F	Prob(F)
Total	31	8046621.875000			
Treatment	15	4592071.875000	306138.125000	1.418	0.2479
Error	16	3454550.000000	215909.375000		

In this case, a statistical model based on the design of the experiment is not the 'best' model.

Analysis of Variance

Randomized Complete Block (RCB) Least square estimation AOV For CHYCI Pyr

Source	DF	Sum of Squares	Mean Square	F	Prob(F)
Total	31	8046621.875000			
Replicate	1	65703.125000	65703.125000	0.291	0.5976
Treatment	15	4592071.875000	306138.125000	1.355	0.2818
Error	15	3388846.875000	225923.125000		

$$F = \frac{\text{Replicate MS}}{\text{Error MS}} = \frac{\sigma^2 + t\sigma^2_r}{\sigma^2}$$

$$\frac{\sigma^2 + t\sigma^2_r}{\sigma^2} < 1 \Rightarrow t\sigma^2_r < 0$$

The RCB model is not mathematically plausible!

Cochran (1947)

- *There is clearly little hope of obtaining information about the treatment effects unless weights are adjusted for differences in fertility from row to row. The adjustment may be made by covariance.*

- *If it were desired to adjust separately for every row, a multiple covariance with four x variables could be computed. … It will be realized that the covariance technique, if misused, can lead to underestimation of errors. It is, however, worth keeping in mind as an occasional weapon for difficult uses.*

…an occasional weapon for difficult uses.

- Where are my letters?

Crop Code		CHYCI
Crop Name		Pyrethrum
Part Rated		HEAD -
Rating Unit		g
Number of Subsamples		1
Trt No.	Treatment Name	1
1	01 01	940.0 -
2	02	1590.0 -
3	A1	1045.0 -
4	A2	965.0 -
5	F1	1930.0 -
6	F2	1000.0 -
7	L1	890.0 -
8	L2	1805.0 -
9	FA1	1430.0 -
10	FA2	1750.0 -
11	LA1	1365.0 -
12	LA2	1930.0 -
13	LF1	1695.0 -
14	LF2	1275.0 -
15	LFA1	1995.0 -
16	LFA2	1620.0 -
LSD P=.05		985.04
Standard Deviation		464.66
CV		32.01

…an occasional weapon for difficult uses.

- Where are my letters?
- *You might have better mean separation if you use a different experimental layout next time.*

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Part Rated	HEAD -
Rating Unit	g
Number of Subsamples	1
Trt No. / Treatment Name	1
1 01 01	940.0 -
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3 A1	1045.0 -
4 A2	965.0 -
5 F1	1930.0 -
6 F2	1000.0 -
7 L1	890.0 -
8 L2	1805.0 -
9 FA1	1430.0 -
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…an occasional weapon for difficult uses.

- Where are my letters?

- *You might have better mean separation if you use a different experimental layout next time.*

- *(This is, we can offer a design-based approach to account for spatial heterogeneity)*

Crop Code		CHYCI
Crop Name		Pyrethrum
Part Rated		HEAD -
Rating Unit		g
Number of Subsamples		1
Trt No.	Treatment Name	1
1	01 01	940.0 -
2	02	1590.0 -
3	A1	1045.0 -
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- Where are my letters?
- *You might have better mean separation if you use a different experimental layout next time.*
- But I want letters now!

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Number of Subsamples	1
Trt No. / Treatment Name	1
1 01 01	940.0 -
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…an occasional weapon for difficult uses.

- Where are my letters?
- *You might have better mean separation if you use a different experimental layout next time.*
- But I want letters now!
- (This is, is there a model-based approach to account for spatial heterogeneity?)

Crop Code Crop Name Part Rated Rating Unit Number of Subsamples		CHYCI Pyrethrum HEAD - g 1
Trt No.	Treatment Name	1
1	01 01	940.0 -
2	02	1590.0 -
3	A1	1045.0 -
4	A2	965.0 -
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14	LF2	1275.0 -
15	LFA1	1995.0 -
16	LFA2	1620.0 -
LSD P=.05 Standard Deviation CV		985.04 464.66 32.01

Letters Now

- Cochran's *occasional weapon for difficult uses* is a rudimentary form of spatial analysis.
- He describes a method of inferring a spatially-varying covariate based on row mean.
- Many other methods for identifying a spatially varying model have been proposed; we consider two general classes.

Spatial Models

- Spatial analysis attempts to recover hidden spatial spatial information. We can think of different degrees of scale or coarseness of these measures. In the context of design trials, these would be
  - Global
    - Identify a spatial pattern encompassing the entire field.
  - Local
    - Analysis of effects in the space adjacent to individual plots.

For more detailed discussion, see e.g. Schabenberger & Pierce 2001 or Plant 2012

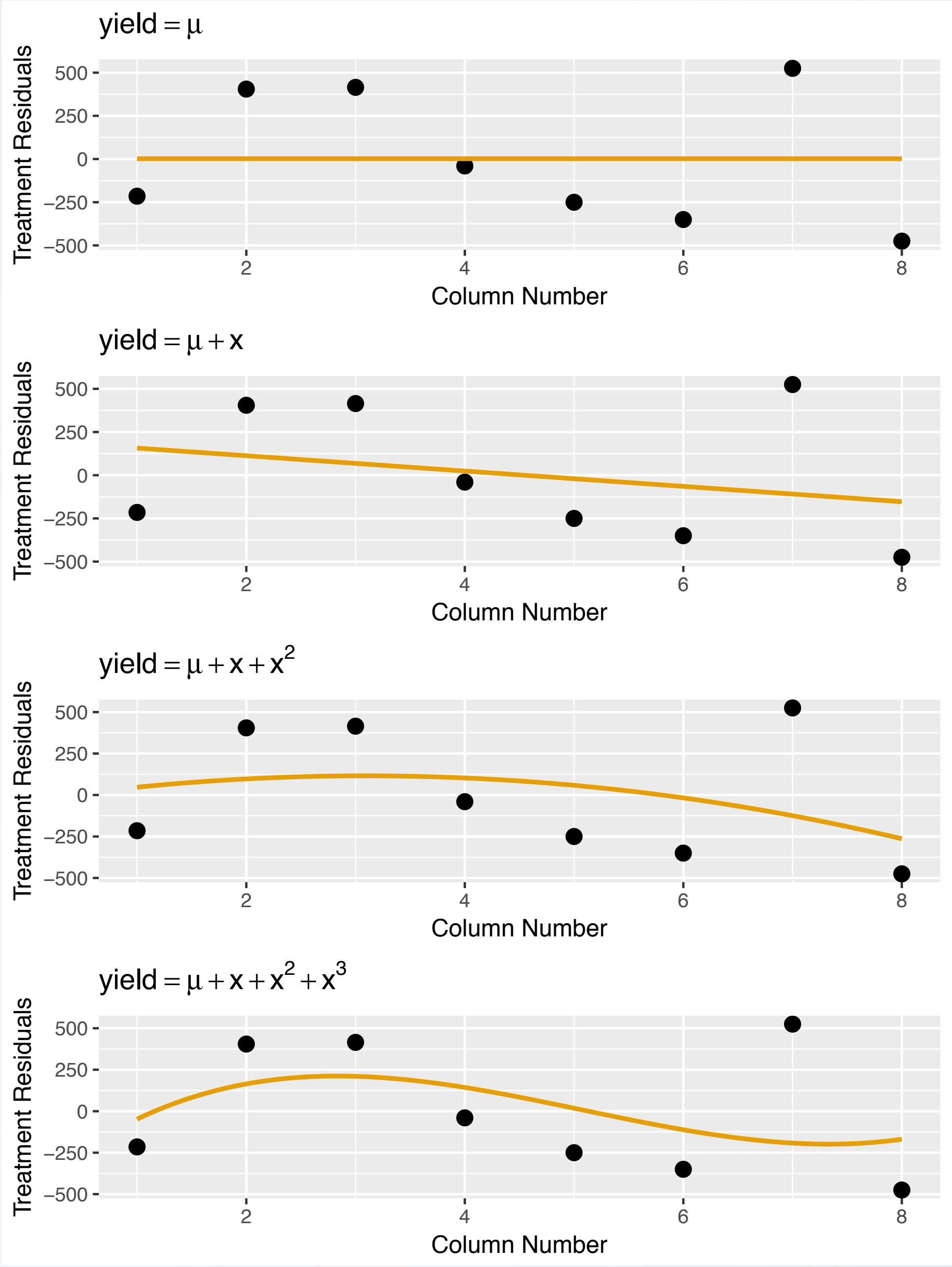
Extremes of Spatial Analysis

- Global (Trend Analysis)
  - We model spatial variability over the entire experiment as a uniformly varying trend.

- Local (Nearest Neighbor Analysis)
  - We model spatial variation by considering the effects of only the nearest neighbor plots.

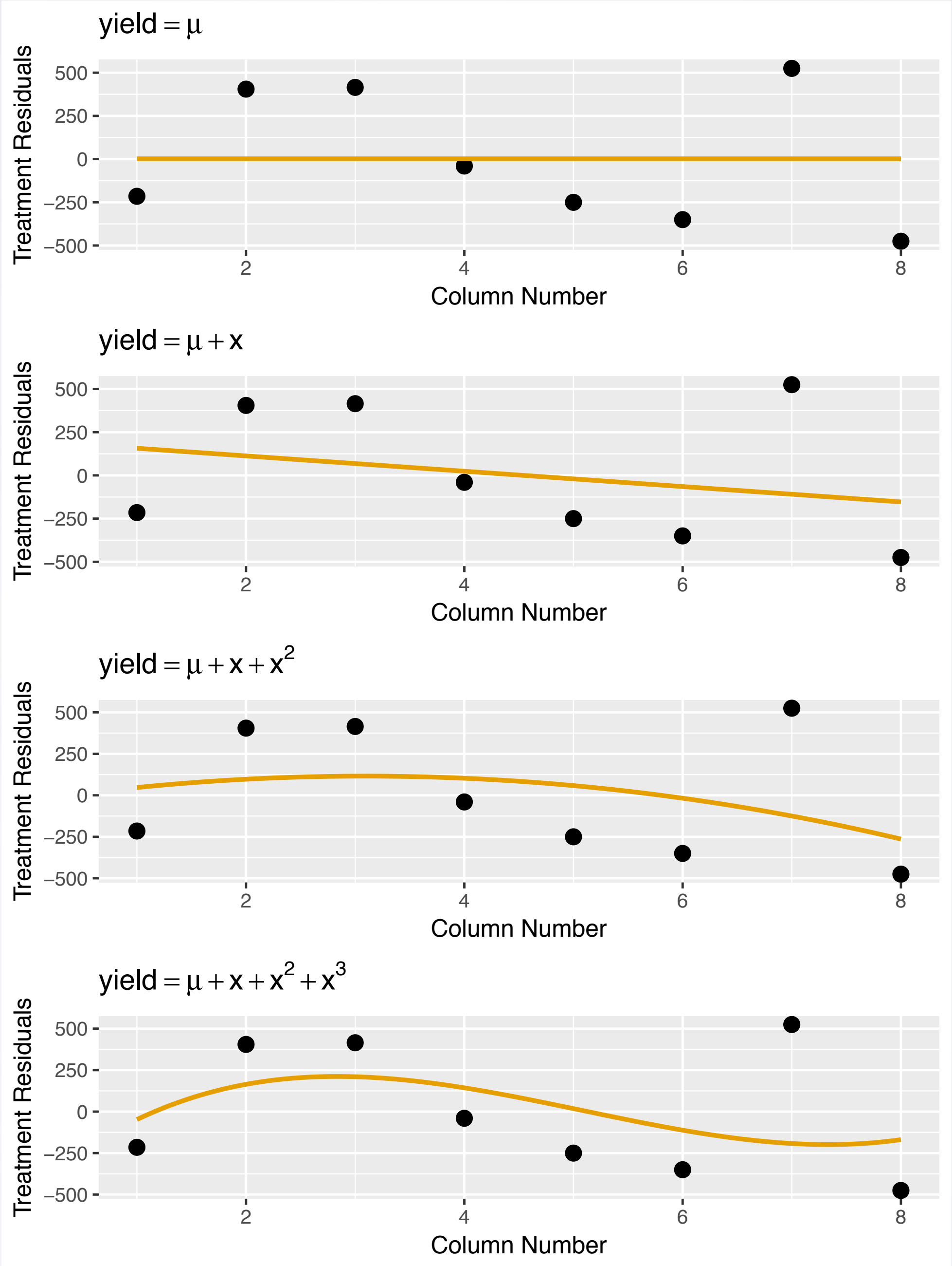
Trend Analysis

- One method to find a global pattern is to use polynomial equations to interpolate between points.
- As we increase the order of a polynomial, we can find a line that varies smoothly with a set of points.



Trend Analysis

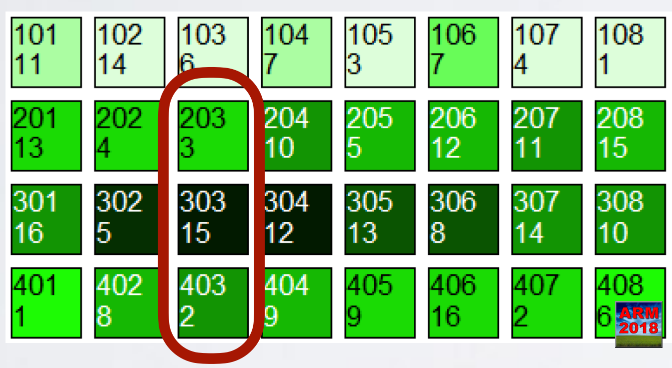
- From top to bottom:
  - Row Mean
  - Linear Trend
  - Quadratic Trend
  - Cubic Trend
- We model both row and column trend simultaneously.



Nearest Neighbor Analysis

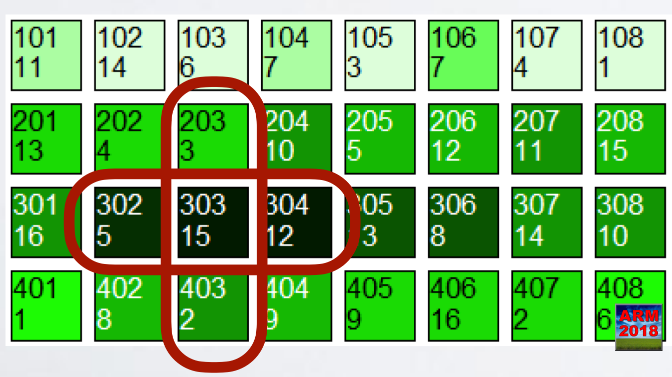
- Papadakis (1937) is credited with the first discussion of using residuals (from treatment means) of neighbor plots as a covariate. There are several variations variations on his method, all falling under the class of nearest neighbor analyses.

Nearest Column Neighbors

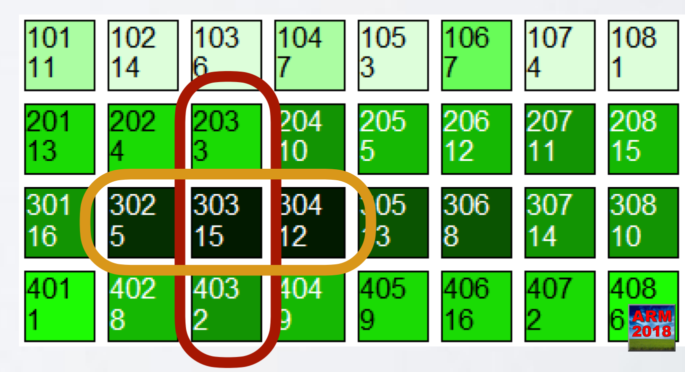


Nearest Row Neighbors

Nearest Row and Column Neighbors (Papadakis)



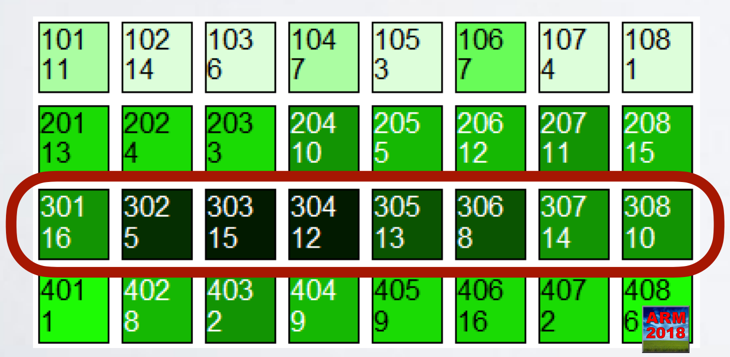
Nearest Row Neighbors and Nearest Column Neighbors

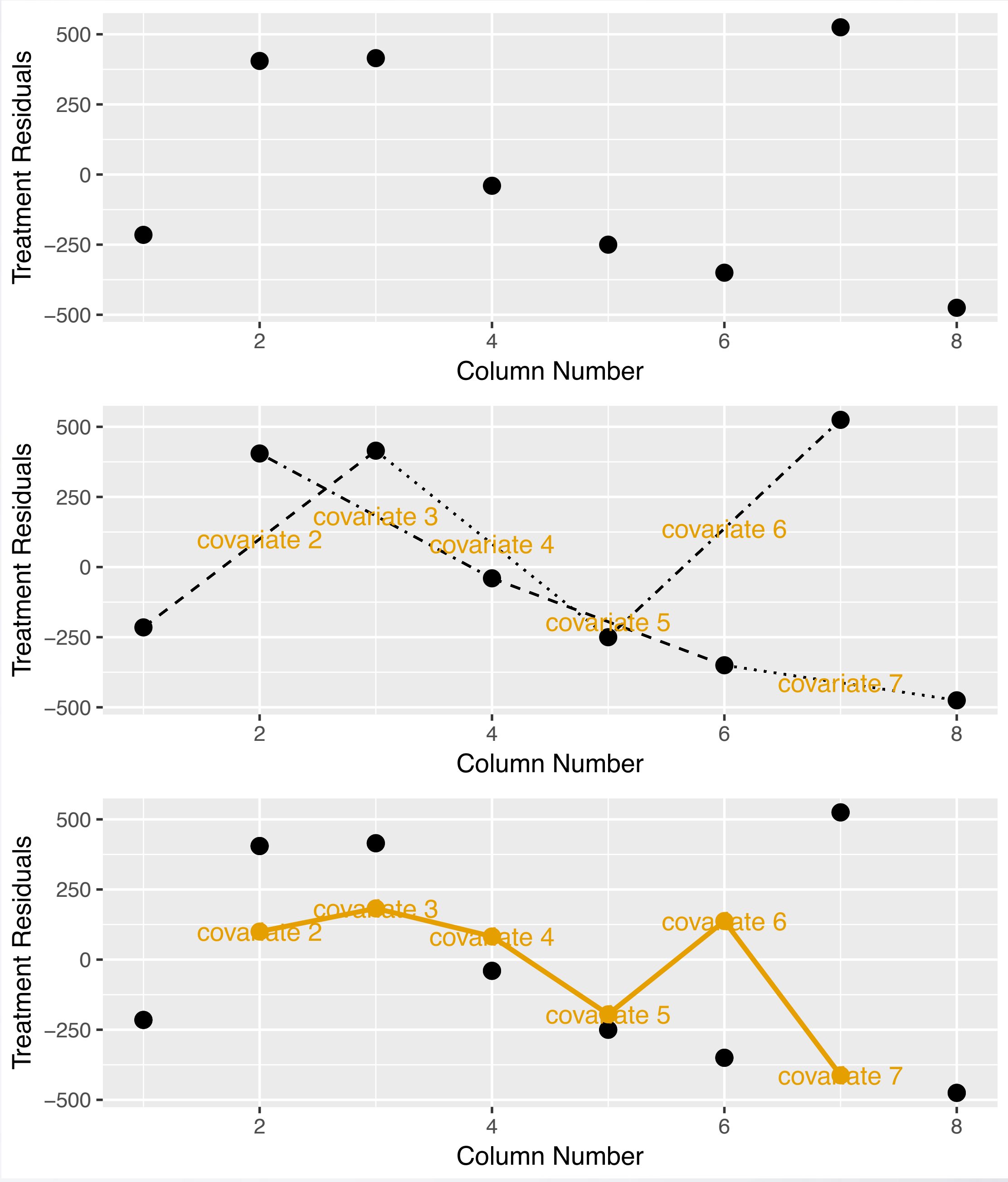


neighbors for plot 303

Nearest Row Neighbors

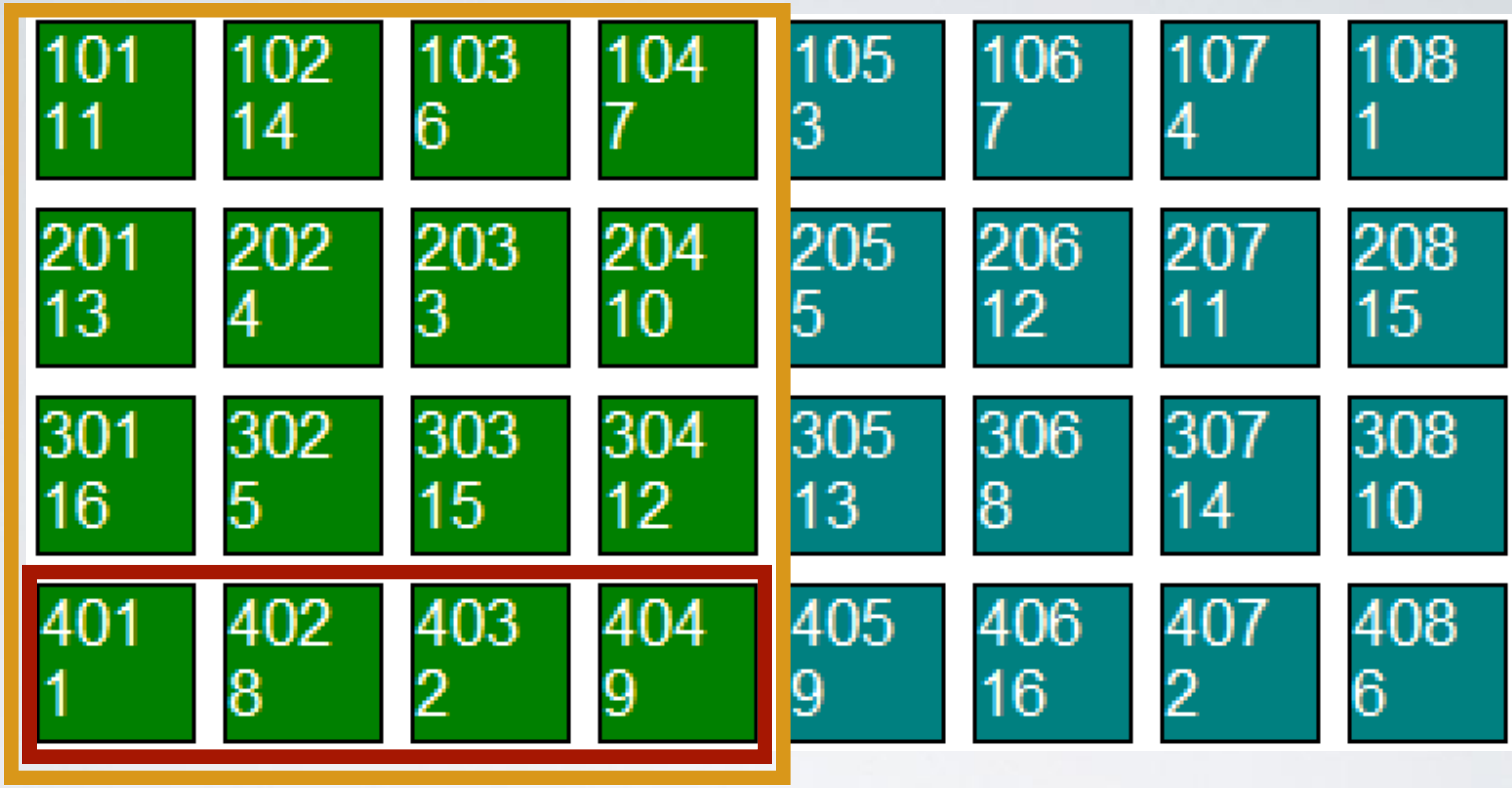
- We compute residuals from treatment means (i.e. CRD model), then find the average of residuals from neighbor plots.
- This average becomes a covariate for plot effect.





Different Experimental Layout

- In this example, spatial variability was found on a scale too small to be captured by replicates (whole blocks).
- We can improve the resolution in blocking by dividing each whole block into smaller, incomplete blocks.
- Incomplete block designs for field trials typically include simple lattices (square, rectangle or alpha-lattices) or row-column lattices (lattice squares).



Incomplete Blocks

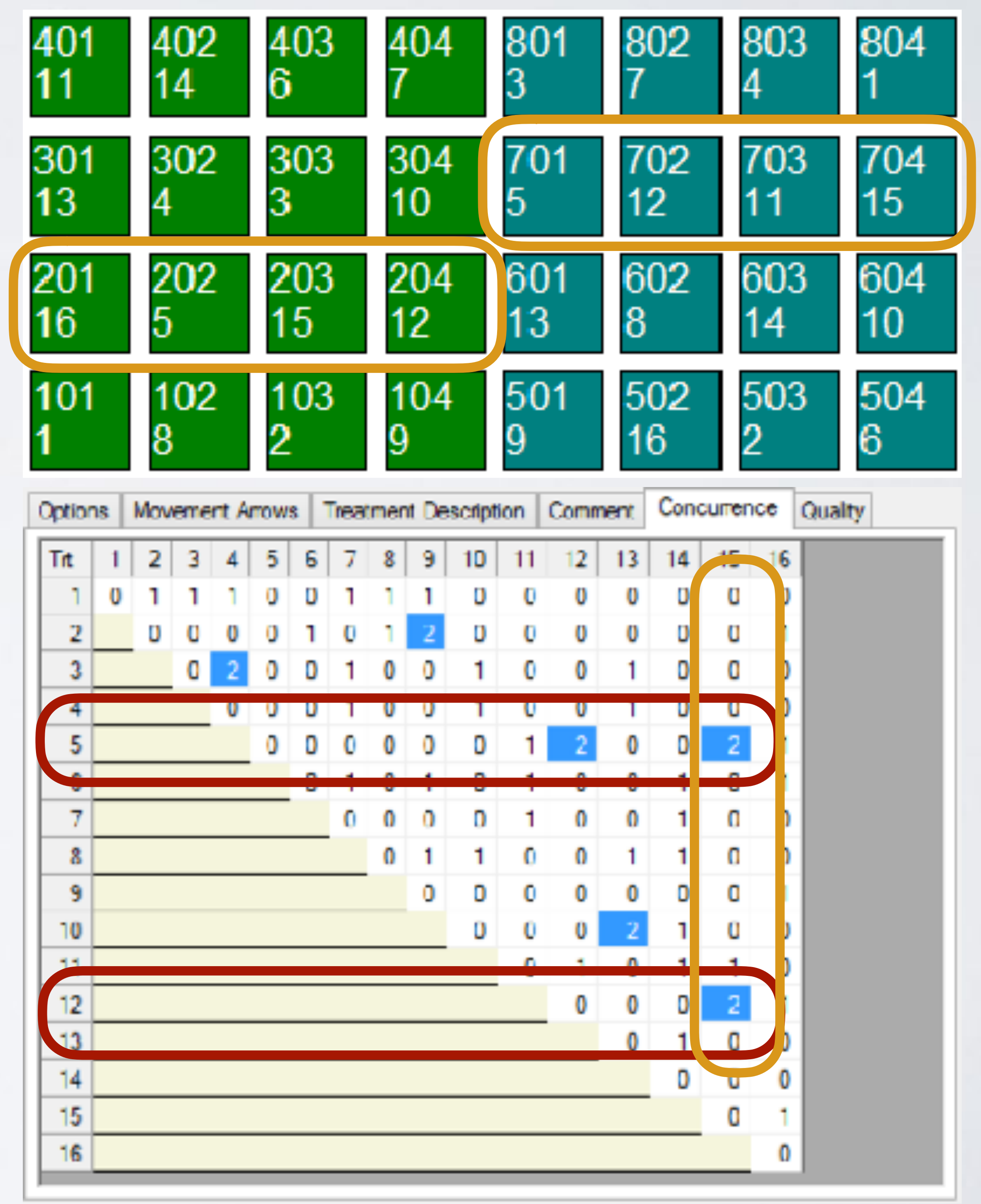
Each replicate constitutes a whole block; rows in replicates can be made into incomplete blocks.

Designing for Spatial Heterogeneity

- However, we can't simply analyze incomplete blocks from an experiment executed as an RCB; we must plan for incomplete blocking.
- We estimate whole block effects by comparing a block average against the grand mean. This is an unbiased estimate when every treatment is represented in each block
- When blocks are incomplete, block effects and treatment effects are confounded. We can recover block information, if we limit the number of times treatments can appear together in blocks.

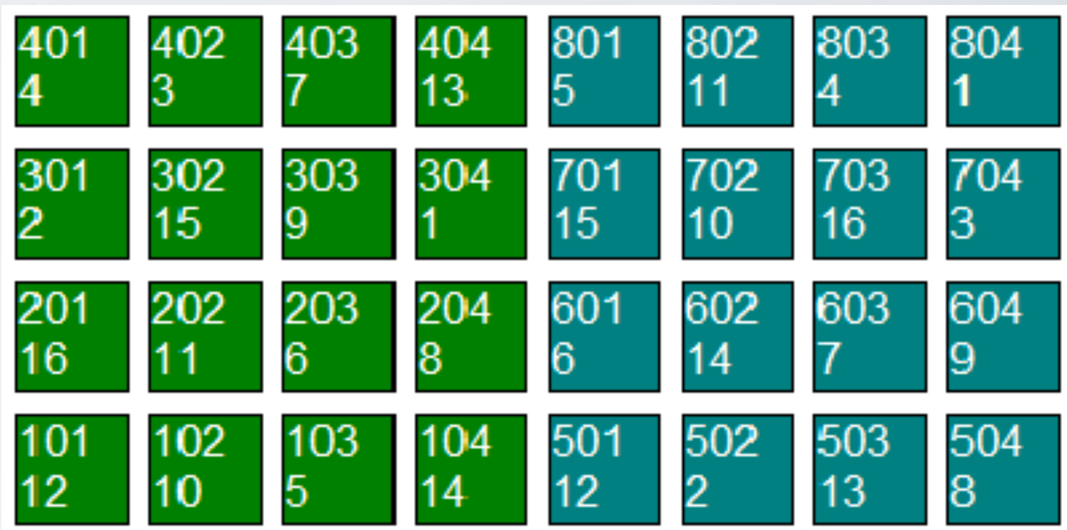
Cochran 1947

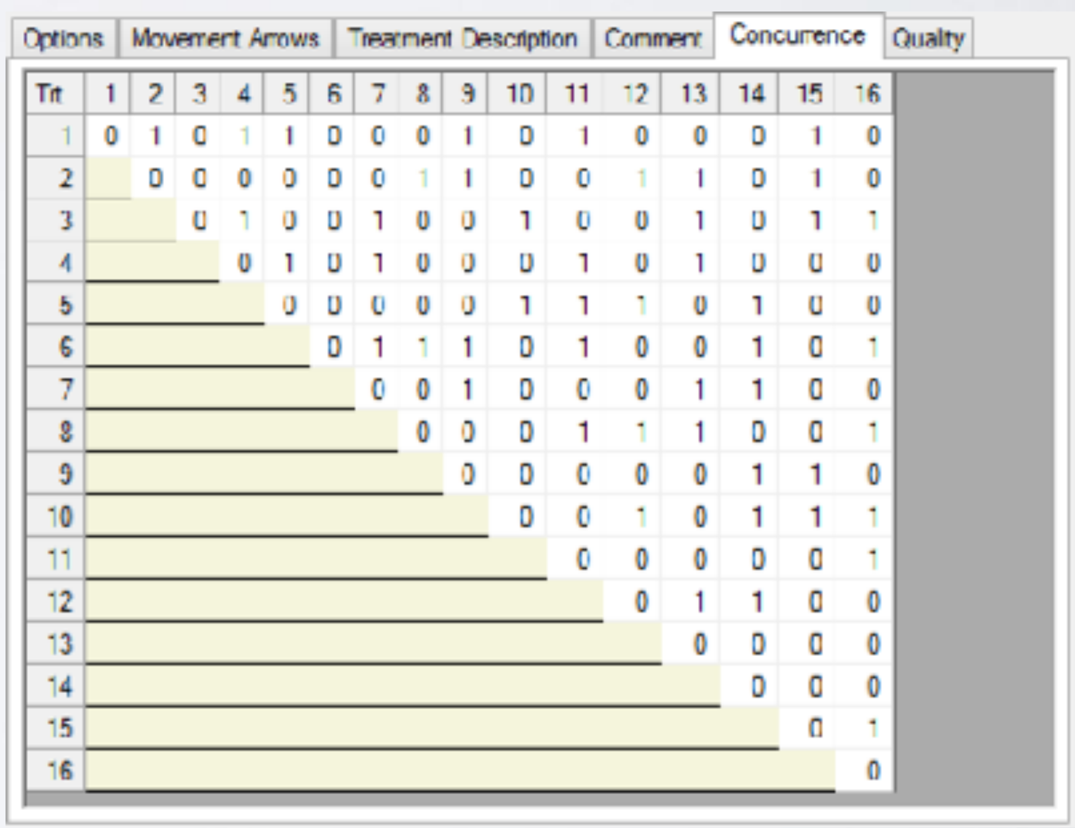
- Since this example was not planned as a lattice design, there are several treatments that appear together in the same block more than once.
- This may introduce a bias in the estimate of block effect
    - In this case if treatment 15 is higher yielding than the other treatments, then we might underestimate the effect of treatments 5 or 12.



Cochran 1947 as Lattice

- The same treatment structure, but randomized as a simple square lattice.
- Each treatment appears exactly one or zero times with any other treatment.
- There still may be a bias in block estimates, but randomization theory allows us to recover information about block variance.





Trt	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0	1	0	1	1	0	0	0	1	0	1	0	0	0	1	0
2		0	0	0	0	0	0	1	1	0	0	1	1	0	1	0
3			0	1	0	0	1	0	0	1	0	0	1	0	1	1
4				0	1	0	1	0	0	0	1	0	1	0	0	0
5					0	0	0	0	0	1	1	1	0	1	0	0
6						0	1	1	1	0	1	0	0	1	0	1
7							0	0	1	0	0	0	1	1	0	0
8								0	0	0	1	1	1	0	0	1
9									0	0	0	0	0	1	1	0
10										0	0	1	0	1	1	1
11											0	0	0	0	0	1
12												0	1	1	0	0
13													0	0	0	0
14														0	0	0
15															0	1
16																0

Design vs Model

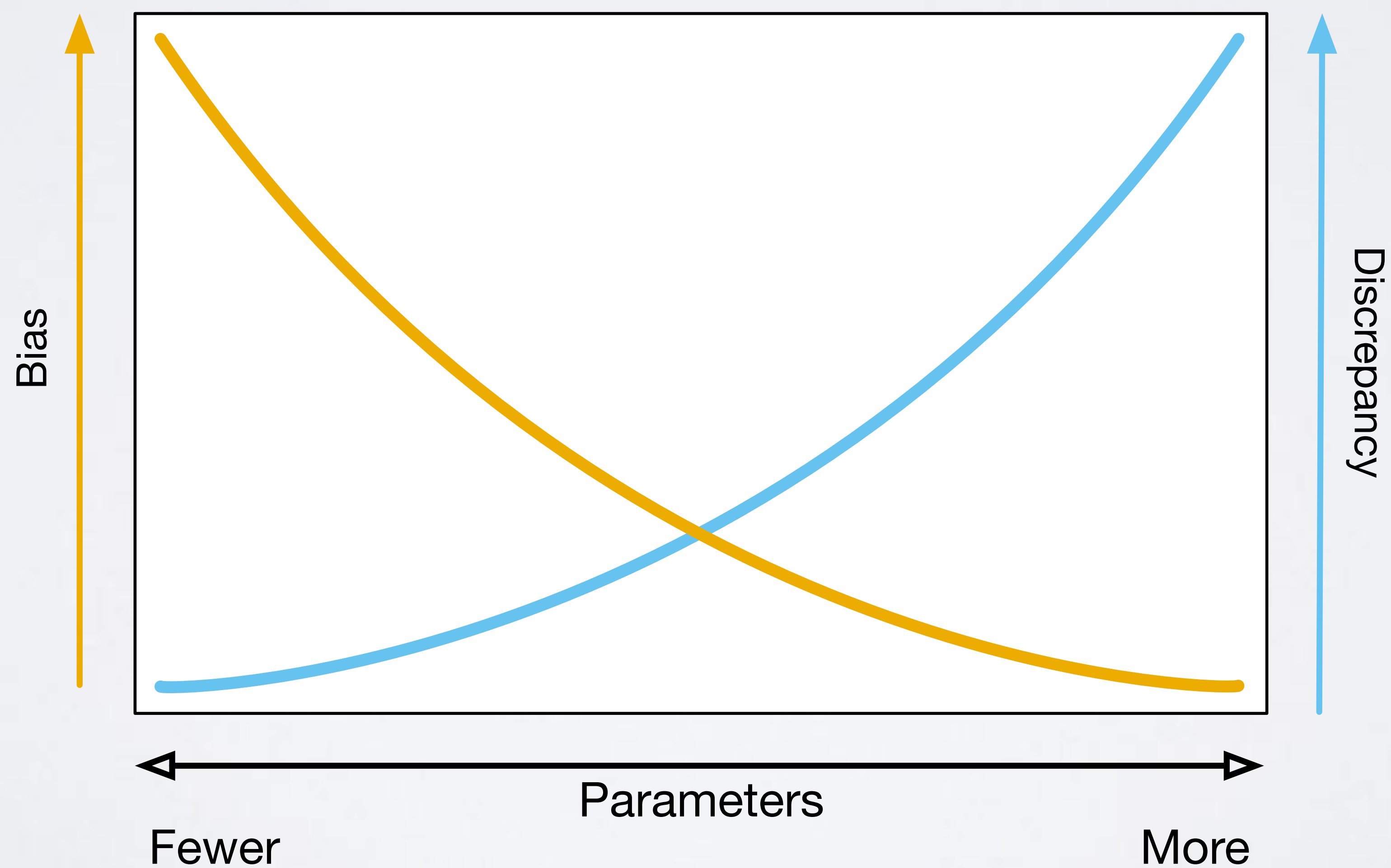
- When faced with an experiment where the design failed to capture spatial information, should we
  - Make the best of the planned design analysis?
    - Randomization theory allows us to make statements about cause-and-effect when we analyze the experiment as designed.
  - Attempt to find a spatial model that can be applied to ***this*** experiment?
    - Modeling limits our ability to discern cause-and-effect, but we may be able to explain the experiment that happened.

Model Selection Problem

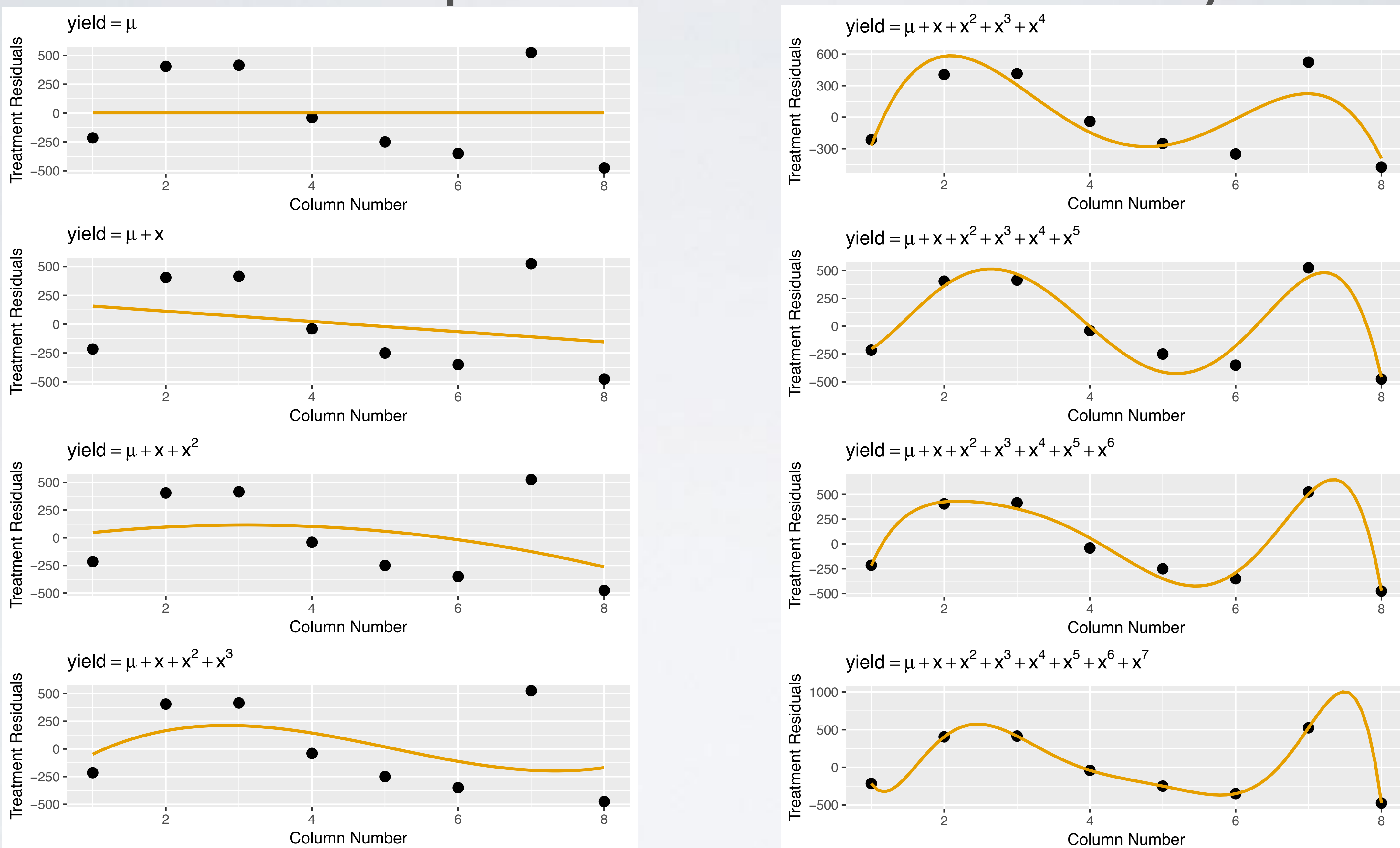
- The original design may not always be the 'best' model, but it will usually be an appropriate model.
- When we detach our analysis from the design, we are faced with the problem of model selection, and we need to determine if a new model is appropriate.
  - The mathematically implausible RCB model for this example is appropriate, in the sense that the inflated error term (relative to CRD) is conservative, and understandable under randomization theory.

Model Selection Problem

- Trade off between bias (underfit) and discrepancy (overfit)



Principle of Parsimony



Entities are not to be multiplied without necessity

Information Criteria

- Akaike (1971) considered that parameters in a linear model are typically chosen to maximize the likelihood, and that log-likelihood is related to a value termed the Kullback-Leibler information number.

- He proposed An Information Criteria that included the number of parameters *k* and the log-likelihood of the model, written as

$$AIC = 2k - 2l\left(\beta, \sigma^2 \middle| y_1, \ldots, y_n\right)$$

- We can simplify to

$$AIC \approx 2k + n\ln\left(RSS\right)$$

AIC/BIC

- AIC should be considered a ***badness-of-fit*** measure.
- A less-bad model reduces Residual SS, while a more-bad model increases the number of parameters. Thus, the choice of model based on AIC is ***smaller is better***

$$AIC \approx 2k + n\ln\left(RSS\right)$$

- Other IC measures, such as the Bayesian IC, incur a different penalty for parameters.

$$BIC \approx \ln(n)k + n\ln\left(RSS\right)$$

Model	RMS	AIC	BIC
Randomized Complete Block	225,923	497.06	523.44
Completely Random	215,909	495.68	520.59
Nearest Column Neighbors	230,104	497.65	524.03
Nearest Row Neighbors	155,257	485.06	511.44
Papadakis Neighbors	158,462	485.71	512.09
Nearest Row/Column Neighbors	163,178	486.44	514.29
Linear Trend	116,238	475.59	503.44
Quadratic Trend	26,874	427.01	459.25
Cubic Trend	***5,835***	***371.67***	***409.78***

Model Comparison

Models and IC applied to Cochran 1947 data

Model	RMS	AIC	BIC
Randomized Complete Block	225,923	497.06	523.44
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CRD is a better model than RCB

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All neighbor models that include rows improve upon CRD, and the nearest row neighbor model is the best of the nearest neighbor analyses.

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All trend models improve upon CRD, with the most improvement coming from a cubic trend.

Letters!

- Some Caveats

- AIC/BIC are not test statistics. They are not assigned p-values and should not be considered tests of significance. They should be for model comparison only.

- These tests won't tell us if the model is correct, or even if the model will be correct for similar experiments.

Crop Code		CHYCI
Crop Name		Pyrethrum
Part Rated		HEAD -
Rating Unit		g
Number of Subsamples		1
Trt No.	Treatment Name	1
1	01 01	940.0 h
2	02	1590.0 de
3	A1	1045.0 gh
4	A2	965.0 h
5	F1	1930.0 ab
6	F2	1000.0 gh
7	L1	890.0 h
8	L2	1805.0 abc
9	FA1	1430.0 def
10	FA2	1750.0 bcd
11	LA1	1365.0 efg
12	LA2	1930.0 ab
13	LF1	1695.0 cd
14	LF2	1275.0 fg
15	LFA1	1995.0 a
16	LFA2	1620.0 cd
LSD P=.05		180.62
Standard Deviation		76.39
CV		5.26
Randomized Complete Block (RCB) AIC		497.0606
Spatial AIC		SPa 371.6681

Visualizing Field Fertility

- Assume we have fit a statistical model to data
- We generate plot level estimates using the fitted model.
- To visualize fertility, we make predictions for a uniformity trial, and replace each plot treatment with a single check treatment.
- The predicted values then show plot values where differences are determined by field fertility estimated from other terms in the model.

Inferred Fertility

Original Yield

Cubic Trend

Is the ‘best’ model an unbiased estimate of spatial heterogeneity?

Simulations

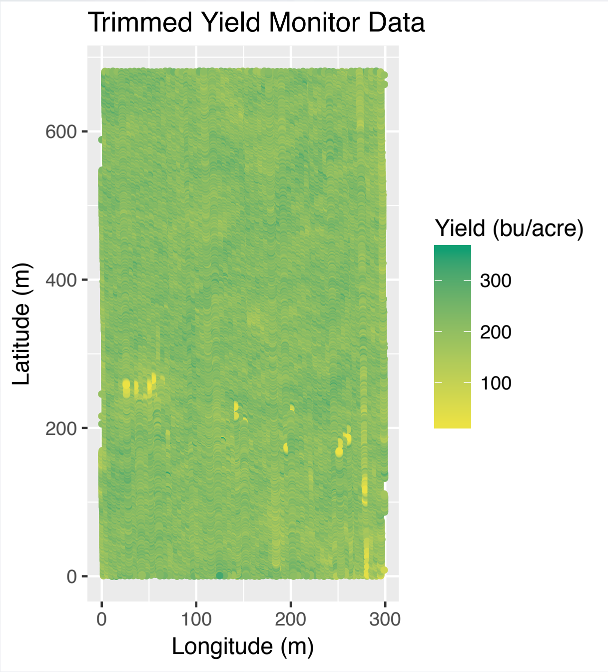
- In this example, RMS, AIC or BIC tended to agree on the choice of 'best' model. This will not always be the case.

- We simulate a series of uniformity trials, using the RCB plan presented in Cochran 1947 and a square lattice based on the same treatment structure.

- Will designing with incomplete blocks lead to a better model in more experiments?

Simulated Experiments

- We overlay trial maps onto yield monitor data to mimic potential spatial heterogeneity.



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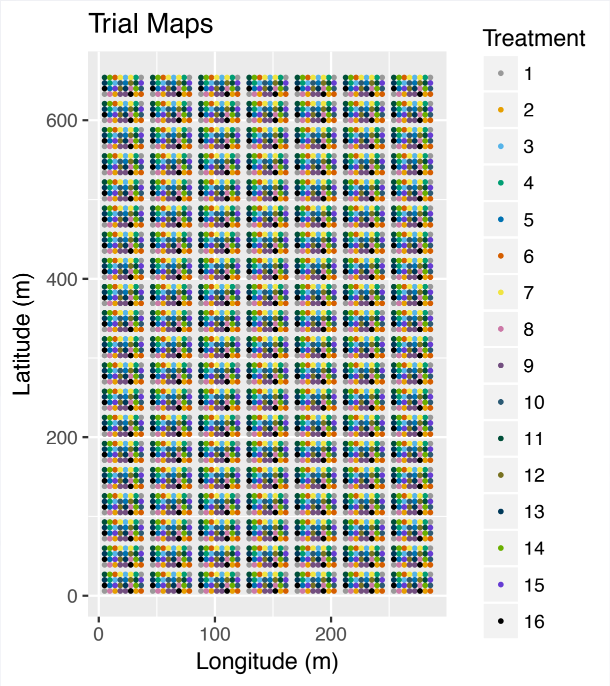

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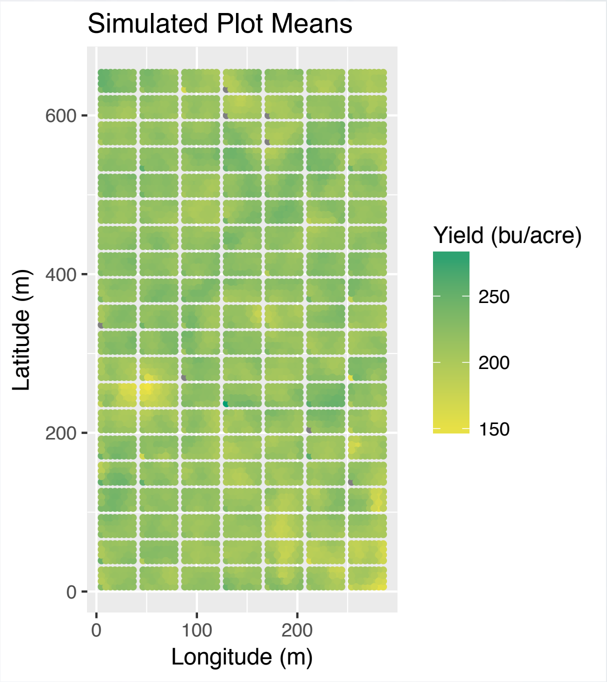

140 simulated uniformity trials

	Design = RCB			Design = Lattice		
Model	RMS	AIC	BIC	RMS	AIC	BIC
CRD	-	-	-	-	-	-
Design	-	-	2	4	4	4
Column NN	-	-	-	1	1	2
Row NN	1	-	-	2	1	4
Papadakis NN	-	-	-	3	2	5
Row/Col NN	1	1	-	1	1	-
Linear Trend	-	-	1	-	-	-
Quadratic Trend	11	2	9	5	2	8
Cubic Trend	127	137	128	124	129	123

Model Selection

Cochran 1947, RCB design, over 140 simulated uniformity trials. Table shows the number of models selected as "best" by each criteria

	Design = RCB			Design = Lattice		
Model	RMS	AIC	BIC	RMS	AIC	BIC
CRD						
Design	-	-	2	4	4	4
Column NN	-	-	-	1	1	2
Row NN	1	-	-	2	1	4
Papadakis NN	-	-	-	3	2	5
Row/Col NN	1	1	-	1	1	-
Linear Trend	-	-	1	-	-	-
Quadratic Trend	11	2	9	5	2	8
Cubic Trend	127	137	128	124	129	123

Cubic trend model is almost always an improvement on the 2-replicate RCB design. AIC chose a cubic trend more often than other criteria.

	Design = RCB			Design = Lattice		
Model	RMS	AIC	BIC	RMS	AIC	BIC
CRD	-	-	-	-	-	-
Design	-	-	2	4	4	4
Column NN	-	-	-	1	1	2
Row NN	1	-	-	2	1	4
Papadakis NN	-	-	-	3	2	5
Row/Col NN	1	1	-	1	1	-
Linear Trend	-	-	1	-	-	-
Quadratic Trend	11	2	9	5	2	8
Cubic Trend	127	137	128	124	129	123

The original design was more often selected when the experiment was executed as a simple lattice.

	Design = RCB			Design = Lattice		
Model	RMS	AIC	BIC	RMS	AIC	BIC
CRD	-	-	-	-	-	-
Design	-	-	2	4	4	4
Column NN	-	-	-	1	1	2
Row NN	1	-	-	2	1	4
Papadakis NN	-	-	-	3	2	5
Row/Col NN	1	1	-	1	1	-
Linear Trend	-	-	1	-	-	-
Quadratic Trend	11	2	9	5	2	8
Cubic Trend	127	137	128	124	129	123

Local (Nearest Neighbor) models were more likely to be selected when the randomization was restricted by incomplete blocking

Cochran and Cox 1957

- Cochran, W. G., & Cox, G. M. (1957). Experimental Design, Table 12.3 - Lattice Square
- Each treatment appears exactly one or zero times with any other treatment in either row or column (within replicates).
- Designs of this type are common examples in the study of spatial models (i.e. Federer 1998, Brownie 1993).

Model	RMS	AIC	BIC
RCB	32.010	494.39	554.64
Row-Column Lattice	***9.575***	***400.82***	521.33
Column Neighbors	21.733	465.83	528.40
Row Neighbor	12.810	426.18	***488.75***
Papadakis Neighbors	14.977	437.90	500.47
Row/Column Neighbors	12.589	425.33	490.22
Linear Trend	25.577	478.50	543.39
Quadratic Trend	21.119	465.29	537.13
Cubic Trend	19.486	460.27	541.39

Model Comparison

Cochran and Cox 1957, RMS, AIC and BIC values for fixed effect linear model.

Model	RMS	AIC	BIC
RCB	32.010	494.39	554.64
Row-Column Lattice	***9.575***	***400.82***	521.33
Column Neighbors	21.733	465.83	528.40
Row Neighbor	12.810	426.18	***488.75***
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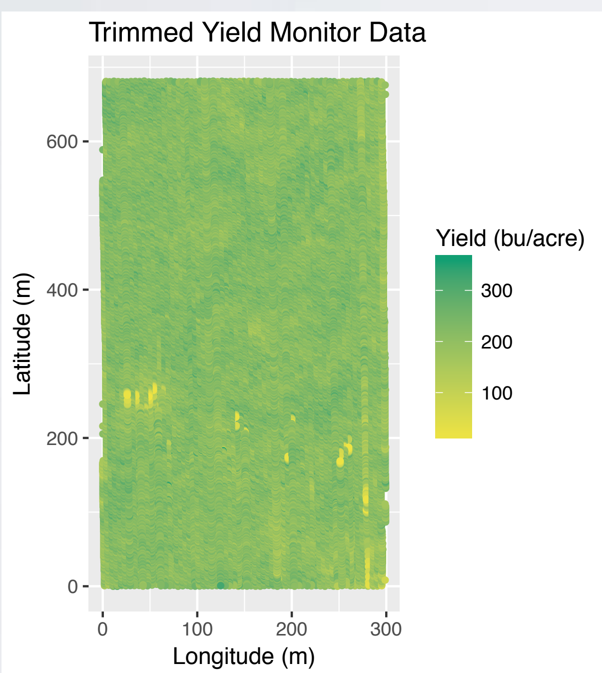
Row/Column Neighbors	12.589	425.33	490.22
Linear Trend	25.577	478.50	543.39
Quadratic Trend	21.119	465.29	537.13
Cubic Trend	19.486	460.27	541.39

RMS and AIC both select the row-column lattice as the best model; BIC, which includes a larger penalty for parameters, chooses the simple Nearest Row Neighbors model.

Simulated Lattice Experiments

- We repeat the uniformity simulations using a row-column lattice.



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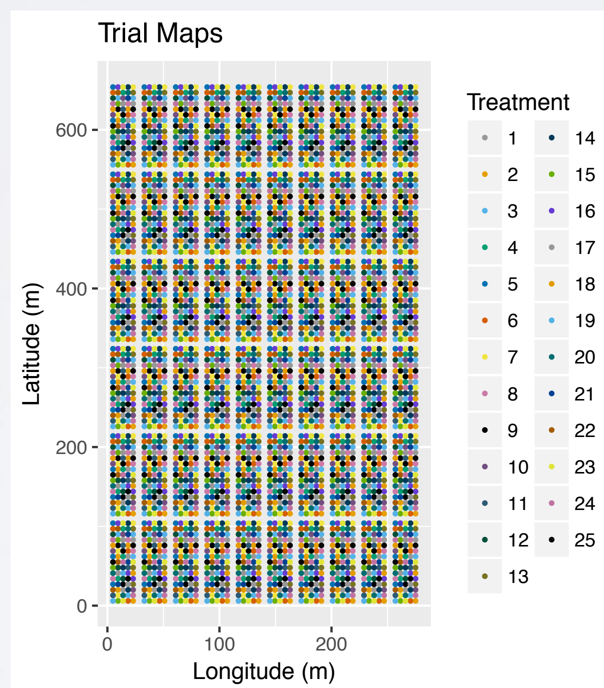

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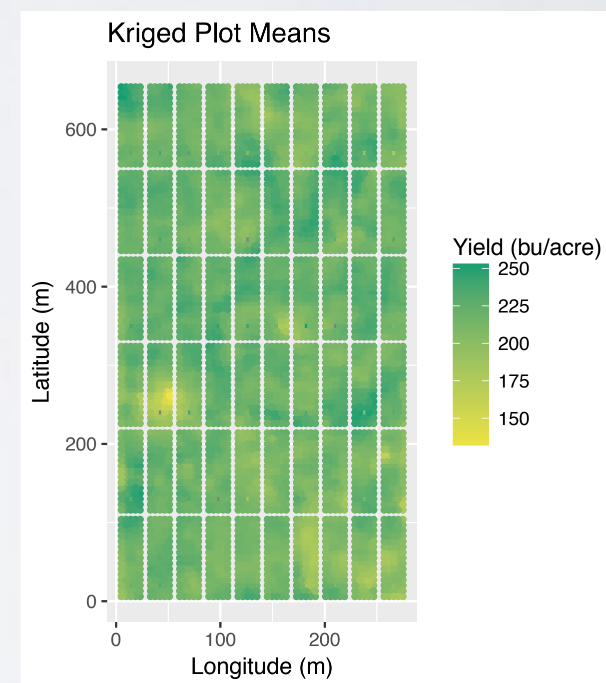

60 simulated uniformity trials

Model	RMS	AIC	BIC
Row-Column Lattice	53	54	13
Nearest Column Neighbors	-	-	1
Nearest Row Neighbors	-	-	-
Papadakis Neighbors	4	4	42
Nearest Row/Column Neighbors	1	1	1
Linear Trend	-	-	-
Quadratic Trend	-	-	1
Cubic Trend	2	1	2

BIC tends to prefer simpler models, in this case when the designed experiment has many parameters.

Spatial Models and MET

- Multi-environment trials are common tools in agricultural research to study treatment by environment interactions.
- We use as example a set of data from the SDSU AES Winter Wheat Variety Trials.

	Yield/Test Weight			
	2003	2004	2005	2006
Location A	NN / RCB	NN / Trend	Trend / Trend	Trend / NN
Location B	NN / RCB	NN / Trend	-	NN / Trend
Location C	Trend / Trend	Trend / Trend	Trend / NN	NN / NN
Location D	Trend / NN	NN / Trend	NN / Trend	Trend / NN
Location E	NN / RCB	NN / Trend	NN / NN	NN / Trend
Location F	-	NN / Trend	- / Trend	Trend / Trend
Location G	NN / Trend	NN / NN	NN / Trend	NN / Trend

Model Selection

Class of model (RCB, Trend or Nearest Neighbor) for 2 traits from 26 RCB trials of 4 replicates and 30 treatments.

Conclusion

- Spatial analysis is a potentially useful tool for understanding the outcome of single field experiments.
- Spatial analysis requires careful selection of the appropriate spatial model.
- The same spatial model might not be applicable to repetitions of the same experimental design, or to different measurements within the same experiment.
- Planning for spatial heterogeneity by using incomplete blocks will more likely allow us to retain our original design.

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