Formal Diagnostics for Modelling Spatial Processes in Field Trials

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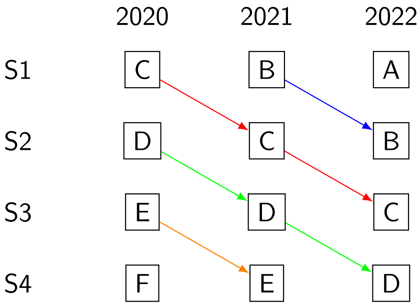
Introduction

An Introduction to Plant Breeding Programs

- The aim of plant breeding programs is to release varieties which are superior for traits of interest such as harvest yield.
- The breeding cycle spans 8-10 years between initial crosses and variety release.
- Lines are evaluated for harvest yield in field trials. Note the terms; lines, varieties and genotypes are used throughout synonymously.

An Introduction to Plant Breeding Programs

- A breeding program involves evaluation in multiple stages i.e. stage 1, stage 2, stage 3 & stage 4, with selection decisions made between stages in each year.
- Only the top performing lines are progressed into the next stage.
  S1: 1000 lines → S2: 300 lines
  → S3: 100 lines → S4: 60 lines
- There are multiple cycles occurring, with a new cohort of lines entering S1 each year.



Introduction

- Selection decisions are based on multi-environment trials (METs), which are selection experiments conducted across various locations and years. We define environments as year and location combinations
- The design of a selection experiment is dependent on the respective stage.
- METs are an important tool in plant breeding to measure genotype by environment interaction. As genotypes vary in their response to different environments.
- A critical component in the analyses of METs is appropriately accounting for spatial heterogeneity within an environment.

Current Frameworks for Modelling Spatial Processes

- There is a rich history of literature for the spatial modelling for field trials such as Papadakis (1937), Bartlett (1978), Zimmerman & Harville (1991), Cullis & Gleeson (1991) etc.
- Gleeson & Cullis (1987) suggested that many of the previously used methods could be generalised as autoregressive integrated moving average (ARIMA) processes.
- Martin (1990) proposed the use of time series models and methods in the analysis of field trials.
  - Including the use of separable lattice processes in the row and column directions.
  - The examination of autocovariances of residuals as diagnostics for model fit and checking model assumptions.
  - Use of different residuals for diagnostics such as white noise residuals.
- Gilmour et al (1997) introduced a widely used framework for modelling spatial processes in field trials where they partitioned spatial variation into three components; natural variation, global trend and extraneous variation. They proposed the use of the sample variogram as a diagnostic tool to identify global trend and extraneous variation.

Current Frameworks for Modelling Spatial Processes

- Non-stochastic smoothing methods have also been proposed and implemented in the analysis of field trials. Such as in Rodrigeuz-Alvarez et al (2018) where tensor product penalised splines (TPS) were used to account for spatial heterogeneity.
- Gogel et al (2023) empirically compared the use of stochastic ARIMA models with non-stochastic TPS models using the Akaike information criterion (aic). They found that ARIMA models outperformed the TPS models, they strongly recommended using ARIMA models in the analysis of field trials. *As such current work is motivated by these important findings!*
- Since Gilmour et al (1997) little work has been done on diagnostics for spatial modelling in field trials.
- An exception is Verbyla (2019) whom highlighted the need to use aic and Bayesian information criterion (bic) for formal model selection.
- The aim of current work is to revisit ideas of Martin (1990) and more recent work of Scaccia & Martin (2005) and Lu & Zimmerman (2004) whom investigated tests of simplifying assumptions of rectangular lattice processes.
  - We note these tests were examined for very simple models (e.g. constant mean and exclusion of random effects).

Some Notation...

The yield data for a field trial is observed on an $n_1 \times n_2$ rectangular (regular) lattice with rows indexed as $i = 1, .., n_1$ and columns (or ranges) indexed by $j = 1, ..., n_2$. In matrix notation we write

$$\boldsymbol{Y} = \begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,n_2-1} & y_{1,n_2} \\ y_{2,1} & y_{2,2} & \cdots & y_{2,n_2-1} & y_{2,n_2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ y_{n_1,1} & y_{n_1,2} & \cdots & y_{n_1,n_2-1} & y_{n_1,n_2} \end{bmatrix}$$

so that $\text{vec}(\boldsymbol{Y}) = \boldsymbol{y}$ is an n-vector with (with $n = n_1 \times n_2$) of the form

$$\boldsymbol{y} = \begin{bmatrix} y_{1,1} \\ y_{2,1} \\ \vdots \\ y_{n_1-1,n_2} \\ y_{n_1,n_2} \end{bmatrix}.$$

Models Used in Current Frameworks

Models used for the analysis of a single field trial are often of the form

$$\boldsymbol{y} = \boldsymbol{X\tau} + \boldsymbol{Z_g u_g} + \boldsymbol{Z_b u_b} + \boldsymbol{Z_p u_p} + \boldsymbol{e},$$

with $\boldsymbol{\tau}$ as the vector of fixed effects, $\boldsymbol{u_g}$ as the vector of genetic effects, $\boldsymbol{u_b}$ as the vector of blocking effects, $\boldsymbol{u_p}$ as the vector of peripheral effects with respective design matrices. Formally we regard the errors to be a realisation of a regular (rectangular) lattice process, so that the indexing set L is such that $L \subset \mathbb{N}^2$. With

$$\boldsymbol{E} = \begin{bmatrix} e_{1,1} & e_{1,2} & \cdots & e_{1,n_2-1} & e_{1,n_2} \\ e_{2,1} & e_{2,2} & \cdots & e_{2,n_2-1} & e_{2,n_2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ e_{n_1,1} & e_{n_1,2} & \cdots & e_{n_1,n_2-1} & e_{n_1,n_2} \end{bmatrix},$$

so that

$$\text{vec}(\boldsymbol{E}) = \boldsymbol{e} = \begin{bmatrix} e_{1,1} \\ e_{2,1} \\ \vdots \\ e_{n_1-1,n_2} \end{bmatrix}.$$

Specification of Random Effects and Errors

The joint distribution of $[\ \boldsymbol{u_g}^\top \quad \boldsymbol{u_b}^\top \quad \boldsymbol{u_p}^\top \quad \boldsymbol{e}^\top\ ]^\top$ is

$$\begin{bmatrix} \boldsymbol{u_g} \\ \boldsymbol{u_b} \\ \boldsymbol{u_p} \\ \boldsymbol{e} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \boldsymbol{G_g}(\boldsymbol{\sigma_g}) & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{G_b}(\boldsymbol{\sigma_b}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{G_p}(\boldsymbol{\sigma_p}) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{R}(\boldsymbol{\phi}) \end{bmatrix} \right).$$

- The genetic variance matrix $\boldsymbol{G_g}(\boldsymbol{\sigma_g})$ is often partitioned into additive and non-additive genetic variance matrices using pedigree or genomic information.
- The variance matrices for blocking and peripheral effects $\boldsymbol{G_b}(\boldsymbol{\sigma_b})$ and $\boldsymbol{G_p}(\boldsymbol{\sigma_p})$ are usually specified as direct sums of scaled identity matrices.
- The form of the residual error variance matrix $\boldsymbol{R}(\boldsymbol{\phi})$ is specified by the covariance function $C(.,.)$.

The predicted errors are $\tilde{\boldsymbol{e}} = \boldsymbol{y} - \{\boldsymbol{X}\hat{\boldsymbol{\tau}} + \boldsymbol{Z_g}\tilde{\boldsymbol{u}}_{\boldsymbol{g}} + \boldsymbol{Z_b}\tilde{\boldsymbol{u}}_{\boldsymbol{b}} + \boldsymbol{Z_p}\tilde{\boldsymbol{u}}_{\boldsymbol{p}}\}$ where $\boldsymbol{X}\hat{\boldsymbol{\tau}}$ is the vector of fitted fixed effects which is unique and $\tilde{\boldsymbol{u}}_{\boldsymbol{g}}$, $\tilde{\boldsymbol{u}}_{\boldsymbol{b}}$, $\tilde{\boldsymbol{u}}_{\boldsymbol{p}}$ are the empirical best linear unbiased estimates of the respective random effects.

Current Frameworks for spatial modelling

The specification of model fixed effects $\boldsymbol{X\tau}$, peripheral effects $\boldsymbol{Z_p u_p}$ and the errors $\boldsymbol{e}$ is determined after fitting a preliminary baseline model. In the baseline model:

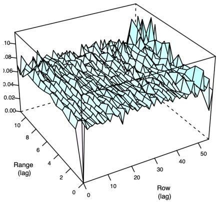
- The fixed effects comprise of simply the overall mean.
- The genetic effects are partitioned into additive and non-additive.
- The blocking effects stay true to the design.
- The vector of errors $\boldsymbol{e}$ is often specified with a separable AR1$\times$AR1 variance structure to model natural variation.
- Usually no peripheral effects are specified.

Visual diagnostics of the predicted errors from the baseline model such as the sample variogram and residual plots are used to diagnose extraneous variation and global trend. For formal model selection procedures various tests may be implemented such as likelihood ratio tests for nested models, wald tests for fixed effects and comparison of aic for (non-nested) models with different fixed effects.

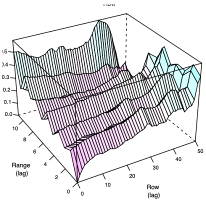
The Sample Variogram in the Current Framework

- The ordinates of the sample variogram $\widehat{V}(g_1, g_2)$ for the residuals are essentially calculated using the average of half the squared difference between pairs of predicted errors at different pairs of lags g_1 and g_2 in the row and column directions. Note there are some adjustments for the sampling distribution of $\widetilde{\boldsymbol{e}}$.
- The sample variogram has a complex asymptotic sampling theory since the ordinates are correlated (Scaccia & Martin, 2005).
- The theoretical variogram for an AR1*x*AR1 process has a smooth appearance and increases exponentially in the row and column lag directions to the variance of the process (Stringer et al 2012). Departures from a smooth appearance may indicate the presence of extraneous variation. For example from experimental procedures like serpentine harvesting saw tooth like patterns may be seen across a direction of lags in the sample variogram.

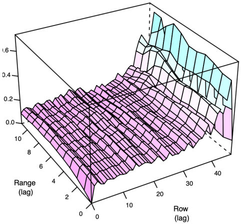
The Sample Variogram: Some Examples



No obvious trend??



Indicative of Range Effects



Indicative of Row Effects

The drawbacks

- Although the sample variogram has some useful properties in terms of identifying the presence of extraneous variation it is purely visual and does not admit a formal assessment of validity of the assumptions of the current variance model, that is second order stationarity, axial symmetry and separability.

Formal Diagnostics for Modelling Spatial Processes

- Spatial modelling for field trials can be difficult and interpretation of informal diagnostics can lead to large disparities in the final models fitted by different practitioners.
- Currently there is a gap in the literature with no formal tests to check model assumptions. Including (i) stationarity, (ii) axial symmetry and (iii) separability.
- The remainder of this talk presents our approach to developing a more formal approach which examines some of these issues in detail.
- To address this we are investigating formal diagnostics to provide a more vigorous frame work for spatial modelling. We also want to improve the efficiency of such procedures in pipelines for the analyses of METs.
- In addition we are investigating goodness of fit statistics.
  - In time series analysis there are white noise tests based on the periodogram which are of interest (Diggle, 1990).
  - There are some complexities we are overcoming!
- Scaccia & Martin (2005) and Lu & Zimmerman (2005) previously investigated various tests for properties such as axial symmetry and separability.

The Covariance Function

We assume a second order (weakly) stationary error (lattice) process in two dimensions so that the covariance function is dependent only on the row and column spatial lags denoted g_1 and g_2. For $j = 1, 2$

$$g_j \in \{-n_j + 1, ..., -1, 0, 1, ..., n_j - 1\}.$$

Therefore $C(.,.)$ at lags g_1 and g_2 is

$$C(g_1, g_2) \quad = \quad \operatorname{cov}\left(E_{u,v}, E_{u_+g_1, v+g_2}\right), \tag{1}$$

the covariance function is even so that $C(g_1, g_2) = C(-g_1, -g_2)$. The respective correlation function at lags g_1 and g_2 is $\rho(g_1, g_2) = \frac{C(g_1, g_2)}{C(0,0)}$ and the associated theoretical semi-variogram is

$$\begin{aligned}\gamma(g_1, g_2) = \frac{1}{2}\operatorname{var}\left(E(u, v) - E_{u+g_1, v+g_2}\right) \quad &= \quad C(0, 0) - C(g_1, g_2) &(2)\\ &= \quad C(0, 0)[1 - \rho(g_1, g_2)]. &(3)\end{aligned}$$

The Spectrum of a Stationary Lattice Process

The spectrum also known as the spectral density function for a second order stationary lattice process at frequencies ω_1 and ω_2 is the fourier transform of the covariance function

$$f(\omega_1, \omega_2) = \frac{1}{(2\pi)^2} \sum_{g_1=-\infty}^{\infty} \sum_{g_2=-\infty}^{\infty} C(g_1, g_2) \cos(\omega_1 g_1 + \omega_2 g_2).$$

Given the spectral density the covariance function may be obtained as

$$C(g_1, g_2) = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} f(\omega_1, \omega_2) \cos(\omega_1 g_1 + \omega_2 g_2) d\omega_1 d\omega_2,$$

(Priestley, 1981; Ripley, 1981).

Axial Symmetry Property

A second order stationary process is axial (or reflection) symmetric if the following equivalent conditions are satisfied:

1. $C(g_1, g_2) = C(-g_1, g_2)$ or $\rho(g_1, g_2) = \rho(-g_1, g_2)$ or $\gamma(g_1, g_2) = \gamma(-g_1, g_2)$ $\forall g_1$ and g_2.
2. $f(\omega_1, \omega_2) = f(-\omega_1, \omega_2)$ $\forall \omega_1$ and ω_2.

That is the correlation function, the covariance function, the variogram and the spectrum are symmetric about the axes (Scaccia & Martin, 2005). Axial symmetry is an important, useful property of spatial processes, but this property is rarely tested in the application of spatial analyses to experiments.

Separability Property

A second order stationary two dimensional process is separable if the following equivalent conditions are satisfied:

1. $C(g_1, g_2) = C(g_1, 0)C(0, g_2)$ or $\rho(g_1, g_2) = \rho(g_1, 0)\rho(0, g_2)$ $\forall g_1$ and g_2.
2. $f(\omega_1, \omega_2) = f(\omega_1, 0)f(0, \omega_2)$ $\forall \omega_1$ and ω_2.

That is the covariance structure, correlation and spectral density are determined by the margins. Often processes are assumed to be separable without any formal tests. *An important note is that separability implies axial symmetry.*

The advantage of specifying a two dimensional separable process is that the error variance can be expressed as the Kronecker product of two component matrices such as $\boldsymbol{R} = \boldsymbol{\Sigma_2} \otimes \boldsymbol{\Sigma_1}$. Consequently the inverse is very simple to calculate particularly for the AR1xAR1 process, where an exact form can be specified.

Defining the Periodogram

The periodogram is the sample version of the spectrum, the periodogram ordinate for ω_1 and ω_2 is the fourier transform of the estimated auto-covariances

$$I(\omega_1, \omega_2) \quad = \quad \frac{1}{(2\pi)^2} \sum_{g_1=-n_1+1}^{n_1-1} \sum_{g_2=-n_2+1}^{n_2-1} \widehat{C}(g_1, g_2)[\cos(\omega_1 g + \omega_2 g_2)],$$

(Priestley, 1981; Ripley, 1981). Where $\widehat{C}(g_1, g_2)$ is a sample estimator of the autocovariance function

$$\widehat{C}(g_1, g_2) = \frac{1}{n} \sum_{s(g_1, g_2)} \tilde{e}(u, v)\tilde{e}(u', v').$$

Asymptotic Properties of the Periodogram

For the fourier frequencies ω_{1_j} and ω_{2_k} of the form

$$\omega_{1_j} = \frac{2\pi j}{n_1} \quad \text{and} \quad \omega_{2_k} = \frac{2\pi k}{n_2},$$

where j and k are integers. The asymptotic distribution of the spectrum (Ripley, 1981) is

$$\begin{aligned} \frac{I(\omega_{1_j}, \omega_{2_k})}{f(\omega_{1_j}, \omega_{2_k})} &\rightarrow \text{i.i.d Exp}(1) \\ \mathbb{E}\left(I(\omega_{1_j}, \omega_{2_k})\right) &\rightarrow f(\omega_{1_j}, \omega_{2_k}) \\ \mathrm{var}\left(I(\omega_{1_j}, \omega_{2_k})\right) &\rightarrow f^2(\omega_{1_j}, \omega_{2_k}), \end{aligned}$$

with $\omega_{1_j} \neq 0, \pi$ and $\omega_{2_k} \neq 0, \pi$ and as n_1 and $n_2 \rightarrow \infty$.

Convenient Properties of the Periodogram

- Unlike the sample variogram or sample autocovariances, the periodogram has attractive asymptotic sampling theory since the ordinates for the fourier frequencies are **independent**. They are also easy to compute!
- Intuitively the periodogram ordinates may be written as sums of squares with

$$I(\omega_{1_j}, \omega_{2_k}) \propto \tilde{\boldsymbol{e}}^\top \boldsymbol{P_{jk}} \tilde{\boldsymbol{e}},$$

  with $\boldsymbol{P_{jk}}$ being the projection matrix for frequencies ω_{1_j} and ω_{2_k}.
- It follows that there exists an orthogonal partitioning of the total sums of squares with

$$\tilde{\boldsymbol{e}}^\top \tilde{\boldsymbol{e}} = \tilde{\boldsymbol{e}}^\top \sum_{(\omega_{1_j}, \omega_{2_k}) \in O} \boldsymbol{P}_{jk} \tilde{\boldsymbol{e}},$$

  where O is a set of fourier frequencies corresponding to unique periodogram ordinates. Also,

$$\tilde{\boldsymbol{e}}^\top \tilde{\boldsymbol{e}} = (2\pi)^2 \left[\underbrace{I(0,0) + I(\pi,0)}_{df=1} + \sum_{(\omega_{1_j}, \omega_{2_k}) \in O - \Omega} 2 \underbrace{I(\omega_{1_j}, \omega_{2_k})}_{df=2} + \underbrace{I(0,\pi) + I(\pi,\pi)}_{df=1} \right],$$

  with $\Omega = \{(0,0), (0,\pi), (\pi,0), (\pi,\pi)\}$. We can see that each of the periodogram ordinates for $(\omega_{1_j}, \omega_{2_k}) \in O$ are asymptotically independent.

Testing for Axial Symmetry

Based on these asymptotics Scaccia & Martin (2005) give various statistics to test axial symmetry such as T_1 based on

$$D(\omega_{1_j}, \omega_{2_k}) = \log(I(\omega_{1_j}, \omega_{2_k})) - \log(I(\omega_{1_j}, -\omega_{2_k})).$$

Under the H_0 of axial symmetry the distribution of $D(\omega_{1_j}, \omega_{2_k})$ is logistic with mean of zero and variance $\pi^2/3$. Given the number of appropriate pairs n_p is large enough for the central limit theorem to hold $T_1 = \frac{\bar{D}\sqrt{n_p}}{\sqrt{\pi^2/3}} \to \mathcal{N}(0,1)$. Another test statistic T_3 is based on

$$G(\omega_{1_j}, \omega_{2_k}) = \frac{I(\omega_{1_j}, \omega_{2_k}) - I(\omega_{1_j}, -\omega_{2_k})}{I(\omega_{1_j}, \omega_{2_k}) + I(\omega_{1_j}, -\omega_{2_k})},$$

so that similarly under the H_0 of axial symmetry and given n_p is large enough $T_3 = \bar{G}\sqrt{3n_p} \to \mathcal{N}(0,1)$

Testing for Separability

If the H_0 of axial symmetry is retained, then we regard $I(\omega_{1_j}, \omega_{2_k})$ and $I(\omega_{1_j}, -\omega_{2_k})$ to be sample realisations of the same spectral value $f(\omega_{1_j}, \omega_{2_k})$. (*Note if H_0 of axial symmetry is rejected, then we would also consider the process to be non-separable.*)

Under the H_0 of separability the

$$E(\log(I(\omega_{1_j}, \omega_{2_k})))) \to c_1 + \log(f(\omega_{1_j}, 0))) + \log(f(0, \omega_{2_k}))$$

and the $\mathrm{var}\left(\log(I(\omega_{1_j}, \omega_{2_k})))\right) \to c_2$ with c_1 and c_2 being constant values. Then given axial symmetry testing for separability may be conducted simply using analysis of variance (Scaccia & Martin, 2005).

Source	SS	MS	F Ratio
Mean	$\boldsymbol{I}^\top \boldsymbol{P}_0 \boldsymbol{I}$	$\boldsymbol{I}^\top \boldsymbol{P}_0 \boldsymbol{I}$	
ω_{1_j}	$\boldsymbol{I}^\top \boldsymbol{P}_{\omega_{1_j}} \boldsymbol{I}$	$MS(\omega_{1_j})$	$MS(\omega_{1_j})/\mathrm{MS(residual)}$
ω_{2_j}	$\boldsymbol{I}^\top \boldsymbol{P}_{\omega_{2_j}} \boldsymbol{I}$	$MS(\omega_{2_j})$	$MS(\omega_{2_j})/\mathrm{MS(residual)}$
$\omega_{1_j} \wedge \omega_{2_j}$	$\boldsymbol{I}^\top \boldsymbol{P}_{\omega_{1_j} \wedge \omega_{2_j}} \boldsymbol{I}$	$MS(\omega_{1_j} \wedge \omega_{2_j})$	$MS(\omega_{1_j} \wedge \omega_{2_j})/\mathrm{MS(residual)}$
residual	$\boldsymbol{I}^\top \boldsymbol{P}_{V_t}^{\perp} \boldsymbol{I}$	MS(residual)	

with $\boldsymbol{I}$ being the relevant vector of ordinates.

Goodness of fit statistics using the Periodogram

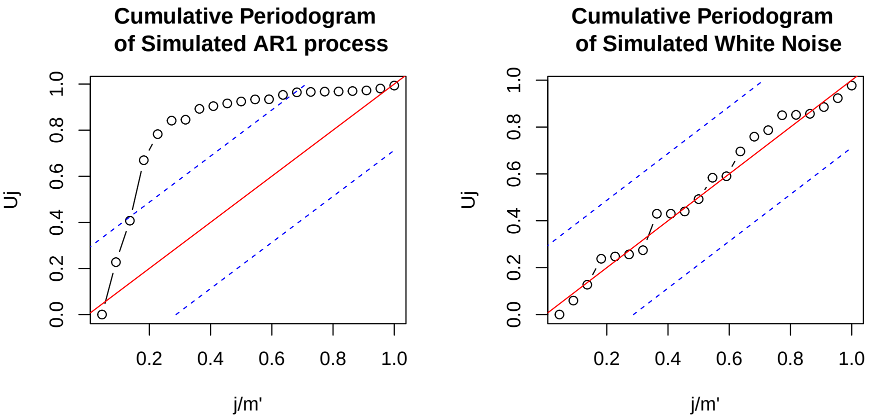
Currently we are looking at various tests to be used as goodness of fit statistics such as white noise tests. We plan to use these tests after examining axial symmetry, separability and second order stationarity.

- For a white noise process e.g. $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \boldsymbol{I})$ the "theoretical" periodogram (spectral density) is a constant function and so the realised periodogram ordinates should only differ because of sampling fluctuations (Diggle, 1990).

The Cumulative Periodogram in 1D

- Essentially the cumulative periodogram is calculated by cumulative summing up the periodogram ordinates such as `cumsum()` in R and dividing by the last cumulative ordinate value.
- For a white noise process the cumulative periodogram should increase approximately linearly. Therefore a test of white noise can be conducted by a statistic which measures departure from linearity (Diggle, 1990).

The Cumulative Periodogram for Simulated One Dimensional Processes $n = 48$.



Current Work

- We are investigating formal diagnostics to provide a more vigorous frame work for spatial modelling in field trials.
  - By investigating statistics for testing assumptions of
    1. Axial Symmetry.
    2. Separability.
  - In this talk we assume second order stationarity, but are looking into diagnostic tests for this.
  - Also assessing statistics for testing goodness of fit.
- The periodogram offers some tests which are simple to implement.
- Although there are some complexities as the sampling distribution of the predicted errors does not have a simple form.
- We are conducting some simulation studies to assess the tests which have been promising. But are not ready to be published.

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Questions?