Available online at www.sciencedirect.com
ScienceDirect
Journal of Statistical Planning and Inference 138 (2008) 93–104
journal of statistical planning and inference
www.elsevier.com/locate/jspi

Robust estimators and designs for field experiments

Douglas P. Wiens[a,*], Julie Zhou[b]

[a]*Department of Mathematical and Statistical Sciences, University of Alberta, Edmonton, Alberta, Canada T6G 2G1*
[b]*Department of Mathematics and Statistics, University of Victoria, Canada*

Available online 16 May 2007

Abstract

We consider the construction of designs for test-control field experiments, with particular attention being paid to the effects of spatial correlation between adjoining plots. In contrast to previous approaches, in which very specific correlation structures were modelled, we explicitly allow a degree of uncertainty on the part of the experimenter. While fitting a particular correlation structure—and variance structure and regression response—the experimenter is thought to be seeking protection against other possible structures in full neighbourhoods of these particular choices. Robustness, in a minimax sense, is obtained through a modification of the kriging estimation procedure, and through the assignment of treatments to field plots.

MSC: Primary 62K05, 62F35; secondary 62P12

Keywords: Check variety; Crop; Kriging; Minimax; Regression; Simulated annealing; Spatial correlation

1. Introduction

We consider the construction of designs for test-control field experiments, with particular attention being paid to the effects of spatial correlation between adjoining plots. These effects are by now well documented—see for example Taplin (1999), Wu and Dutilleul (1999) and Legendre et al. (2004). Martin (1986) initiated a systematic study of designs which account for spatial correlation; see also Petraitis (2001) and Fagroud and Van Meirvenne (2002) for *ad hoc* recommendations. In contrast to these approaches (but see also Martin et al., 1993), in which very specific correlation structures were modelled, we explicitly allow a degree of uncertainty on the part of the experimenter. While fitting a particular correlation structure—and variance structure and regression response—the experimenter is thought to be seeking protection against other possible structures in full neighbourhoods of these choices. Robustness, in a minimax sense detailed below, is obtained through a modification of the kriging estimation procedure, and through the assignment of treatments to field plots.

To motivate the discussion, consider a rectangular layout of plots, with r rows and c columns. There are t crop varieties to be planted. One, denoted variety 1, is a control, or "check" variety. The $n = rc$ locations of plots are denoted by $\mathbf{t}_1, \ldots, \mathbf{t}_n$. A task of the experimenter is to allocate crop varieties to plots, subject perhaps to constraints on the frequencies $\{n_i\}_{i=1}^{t}$ with which each variety will appear; for instance we may require that they be equal, or that the frequency n_1 have special prominence.

* Corresponding author. Tel.: +1 780 492 4406; fax: +1 780 492 6823.
E-mail addresses: doug.wiens@ualberta.ca (D.P. Wiens), jzhou@math.uvic.ca (J. Zhou).

0378-3758/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.jspi.2007.05.020

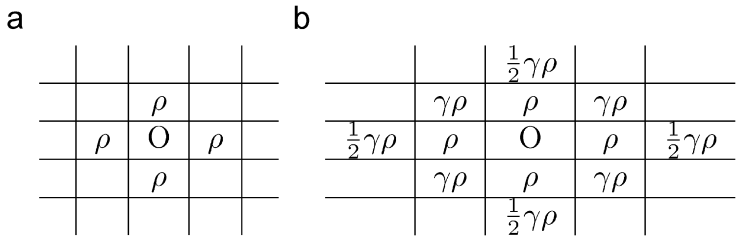

Fig. 1. Correlation structures for plot O: (a) NN(1); (b) MA(1).

In this paper treatments are not limited to crop varieties; they can be various nutrients, or combinations of crop varieties and nutrients, etc. One objective of the experiment is to model an observed random variable Y, e.g. crop yield, in terms of variety, and perhaps in terms of other design variables (added nutrients, water, etc.) as well. Denote by $\mathbf{x}_{q\times 1}$ the vector of such design variables. Each treatment determines a value of $\mathbf{x}$. We might also allow for a deterministic spatial trend. The experimenter intends to fit a linear regression model, with regressors $\mathbf{v}(\mathbf{x})$: $p_1 \times 1$, $\mathbf{w}(\mathbf{t})$: $p_2 \times 1$ and response

$$E[Y|\mathbf{x},\mathbf{t}] \approx \mathbf{v}^{\mathrm{T}}(\mathbf{x})\boldsymbol{\theta}_{(1)} + \mathbf{w}^{\mathrm{T}}(\mathbf{t})\boldsymbol{\theta}_{(2)}. \tag{1}$$

As indicated by (1) the fitted response is acknowledged to be only an approximation, in which case ensuing estimates and predictions will be biased. In some cases, depending on the richness of the space over which $\mathbf{x}$ varies, some protection against this bias can be obtained through a judicious choice of the design variables.

Even in the simple case that $q = 1$ and x is merely the indicator of the variety, the allocation of varieties to plots should take into account the spatial correlations between the plots. Failure to do so may of course result in inefficient estimates. But the specification of an appropriate model for these correlations can be very difficult, and one typically posits a simple and intuitively pleasing model in the hopes that it will at least be adequate, if not particularly accurate. Robustness of design is again called for, as is robustness of the estimation procedure.

We anticipate that the experimenter will work with a particular correlation structure, but seek protection against a full neighbourhood of such structures. Two particular structures, appealing for their simplicity, are the first order nearest neighbour (NN(1)) model (Kiefer and Wynn, 1981) and the first order moving average (MA(1)) model (Haining, 1978). These are illustrated in Fig. 1 (a) and (b), respectively. Under the NN(1) structure the plot O has positive correlation ρ only with its first order neighbours, and $\rho \in (0, \frac{1}{4})$. Under the MA(1) structure O has positive correlation with 12 neighbours, described by a parameter $\gamma \in (0, \frac{1}{4})$ with $\rho = 2\gamma/(1+4\gamma^2)$.

A further call for robustness comes from the need to assume a variance structure on the measurement errors. One would generally fit a homoscedastic model, while wishing for some protection against heteroscedasticity. Again we will deal with this by seeking robustness against a class of such structures.

Specifically and more generally, we have a fixed set $\mathscr{T} = \{\mathbf{t}_1, \ldots, \mathbf{t}_n\}$ of locations of field plots. At location $\mathbf{t}_i$ one sets the levels of an independent variable $\mathbf{x}$, and observes

$$Y_i = E[Y|\mathbf{x}_i, \mathbf{t}_i] + \delta(\mathbf{t}_i) + \varepsilon(\mathbf{t}_i), \quad i = 1, \ldots, n.$$

Here:

(i) $\{\varepsilon(\mathbf{t})|\mathbf{t} \in \mathscr{T}\}$ is a set of uncorrelated zero-mean random errors, with variance matrix $\mathbf{F} = \mathrm{diag}(f(\mathbf{t}_1), \ldots, f(\mathbf{t}_n))$. We allow f to vary over a neighbourhood of a variance function f_0:

$$\mathscr{F}_\alpha = \left\{ f(\cdot) \left| \max_{\mathbf{t}\in\mathscr{T}} \right| f(\mathbf{t}) - f_0(\mathbf{t})| \leqslant \alpha,\ f(\mathbf{t}) \geqslant 0 \right\}.$$

(ii) $\{\delta(\mathbf{t})|\mathbf{t} \in \mathscr{T}\}$ is a zero-mean, spatially correlated stochastic process (uncorrelated with $\{\varepsilon(\mathbf{t})|\mathbf{t} \in \mathscr{T}\}$) with covariance function $g(\mathbf{t}_i, \mathbf{t}_j) = cov[\delta(\mathbf{t}_i), \delta(\mathbf{t}_j)]$ and covariance matrix $\mathbf{G}_{n\times n} = (g(\mathbf{t}_i, \mathbf{t}_j))_{i,j=1}^n$. We allow g to vary over

$$\mathscr{G}_\beta = \{g(\cdot,\cdot)|\mathbf{0} \leqslant \mathbf{G} \leqslant \mathbf{G}^{(0)} + \beta\mathbf{K}\},$$