Optimal design of blocked and split-plot experiments in the presence of autocorrelation

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Linear mixed-effects model

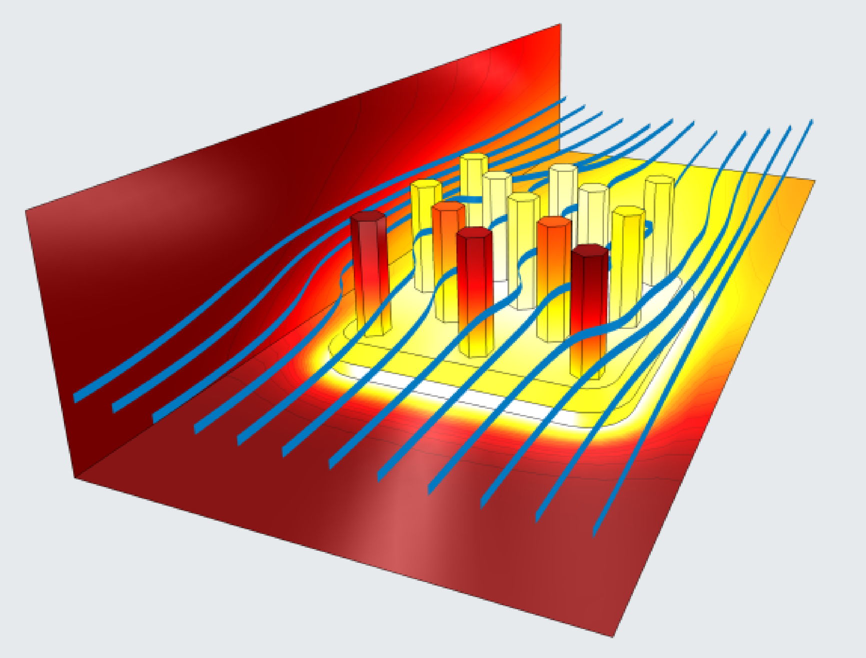
The model for analyzing a blocked/split-plot experiment involving N runs, F factors and K blocks/whole plots is a mixed-effects model of the form

$$\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X})\boldsymbol{\beta} + \boldsymbol{B}\boldsymbol{\delta} + \boldsymbol{\varepsilon},$$

where:

- $\boldsymbol{Y}$ is the $N \times 1$ vector containing the N responses
- $\boldsymbol{X}$ is the $N \times F$ design matrix containing the factor levels for each observation
- $\boldsymbol{\beta}$ is the $P \times 1$ vector containing the P model parameters
- $\boldsymbol{f}(\boldsymbol{X})$ is the $N \times P$ extended design matrix involving the model expansion of the factor levels for each observation
- $\boldsymbol{B}$ is the $N \times K$ matrix that allocates the observations to the blocks/whole plots
- $\boldsymbol{\delta}$ is the $K \times 1$ vector of block/whole-plot effects (which follow a normal distribution $N(0, \sigma^2_\delta)$)
- $\boldsymbol{\varepsilon}$ is the $N \times 1$ vector containing the residual errors of each observation (which follow a normal distribution $N(0, \sigma^2_\varepsilon)$)

Motivation to consider autocorrelation



Simulation of the heat transfer in an industrial oven. Example of spatial autocorrelation

Assumption: observations that are performed closer to each other (in time or space) are more strongly correlated than observations that are performed further apart

Example: experiments involving an industrial oven. The heat transfer in the oven makes the positioning of the observations an important aspect to be considered by an optimal design

Autoregressive correlation structure

The dependence between observations in the k-th block/whole plot $Y_{k1}, \ldots, Y_{kN_k}$ is given by the variance-covariance submatrix

$$\boldsymbol{V}_k = \begin{bmatrix} 1+\eta & \eta & \ldots & \eta \\ \eta & 1+\eta & \ldots & \eta \\ \vdots & \vdots & \ddots & \vdots \\ \eta & \eta & \ldots & 1+\eta \end{bmatrix} + \frac{1}{1-\rho^2} \begin{bmatrix} 1 & \rho & \ldots & \rho^{N_k-1} \\ \rho & 1 & \ldots & \rho^{N_k-2} \\ \vdots & \vdots & \ddots & \vdots \\ \rho^{N_k-1} & \rho^{N_k-2} & \ldots & 1 \end{bmatrix},$$

where:

- η is the variance ratio $\sigma^2_\delta/\sigma^2_\varepsilon$ that measures the extent to which observations in the same block/whole plot are correlated
- ρ is the autoregressive parameter of an AR(1) process. It describes the additional spatial or temporal correlation of observations in the same block/whole plot

$\mathcal{D}$-optimality criterion

The $\mathcal{D}$-optimality criterion seeks to obtain the most precise parameter estimates of the model by maximizing the determinant of the information matrix of the design

$$\mathcal{D}(\boldsymbol{X}) = |\boldsymbol{X}'\boldsymbol{V}^{-1}\boldsymbol{X}|,$$

where:

- $\boldsymbol{V}$ is the variance-covariance matrix of $\boldsymbol{Y}$

In order to compare the quality of two designs $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$, we calculate the $\mathcal{D}$-efficiency of the first design relative to the second one using the expression

$$\mathcal{D}\text{-efficiency}(\boldsymbol{X}_1, \boldsymbol{X}_2) = 100 \left(\frac{\mathcal{D}(\boldsymbol{X}_1)}{\mathcal{D}(\boldsymbol{X}_2)}\right)^{1/P} = 100 \left(\frac{|\boldsymbol{X}_1'\boldsymbol{V}_1^{-1}\boldsymbol{X}_1|}{|\boldsymbol{X}_2'\boldsymbol{V}_2^{-1}\boldsymbol{X}_2|}\right)^{1/P},$$

where:

- $\boldsymbol{V}_1$ and $\boldsymbol{V}_2$ are calculated considering the same values of ρ and η

Optimal designs generated ignoring and considering autocorrelation

- 4 continuous factors and 3 blocks/whole plots of size 4
- Estimation of main-effects models

$$\begin{array}{rrrr} \hline +1 & -1 & +1 & +1 \\ -1 & +1 & -1 & +1 \\ +1 & +1 & -1 & -1 \\ -1 & -1 & +1 & -1 \\ \hline +1 & +1 & +1 & -1 \\ -1 & -1 & -1 & +1 \\ +1 & -1 & -1 & -1 \\ -1 & +1 & +1 & +1 \\ \hline -1 & -1 & +1 & -1 \\ -1 & +1 & -1 & -1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & +1 & +1 \\ \hline \end{array} \qquad \begin{array}{rrrr} \hline +1 & -1 & -1 & -1 \\ -1 & +1 & +1 & +1 \\ +1 & -1 & -1 & -1 \\ -1 & +1 & +1 & +1 \\ \hline +1 & -1 & +1 & +1 \\ -1 & +1 & -1 & -1 \\ +1 & -1 & +1 & +1 \\ -1 & +1 & -1 & -1 \\ \hline +1 & +1 & -1 & +1 \\ -1 & -1 & +1 & -1 \\ +1 & +1 & +1 & -1 \\ -1 & -1 & -1 & +1 \\ \hline \end{array}$$

$\rho = 0$ $\qquad$ $\rho \neq 0$

Optimal designs for a block experiment generated ignoring and considering autocorrelation

$$\begin{array}{rrrr} \hline \mathbf{-1} & -1 & -1 & -1 \\ \mathbf{-1} & +1 & +1 & +1 \\ \mathbf{-1} & +1 & +1 & -1 \\ \mathbf{-1} & -1 & -1 & +1 \\ \hline \mathbf{+1} & -1 & +1 & +1 \\ \mathbf{+1} & +1 & -1 & +1 \\ \mathbf{+1} & +1 & -1 & -1 \\ \mathbf{+1} & -1 & +1 & -1 \\ \hline \mathbf{+1} & -1 & -1 & -1 \\ \mathbf{+1} & +1 & +1 & -1 \\ \mathbf{+1} & -1 & +1 & +1 \\ \mathbf{+1} & +1 & -1 & +1 \\ \hline \end{array} \qquad \begin{array}{rrrr} \hline \mathbf{+1} & +1 & -1 & -1 \\ \mathbf{+1} & -1 & +1 & +1 \\ \mathbf{+1} & +1 & -1 & -1 \\ \mathbf{+1} & -1 & +1 & +1 \\ \hline \mathbf{-1} & -1 & -1 & -1 \\ \mathbf{-1} & +1 & +1 & +1 \\ \mathbf{-1} & -1 & +1 & -1 \\ \mathbf{-1} & +1 & -1 & +1 \\ \hline \mathbf{-1} & -1 & -1 & +1 \\ \mathbf{-1} & +1 & +1 & -1 \\ \mathbf{-1} & -1 & -1 & +1 \\ \mathbf{-1} & +1 & +1 & -1 \\ \hline \end{array}$$

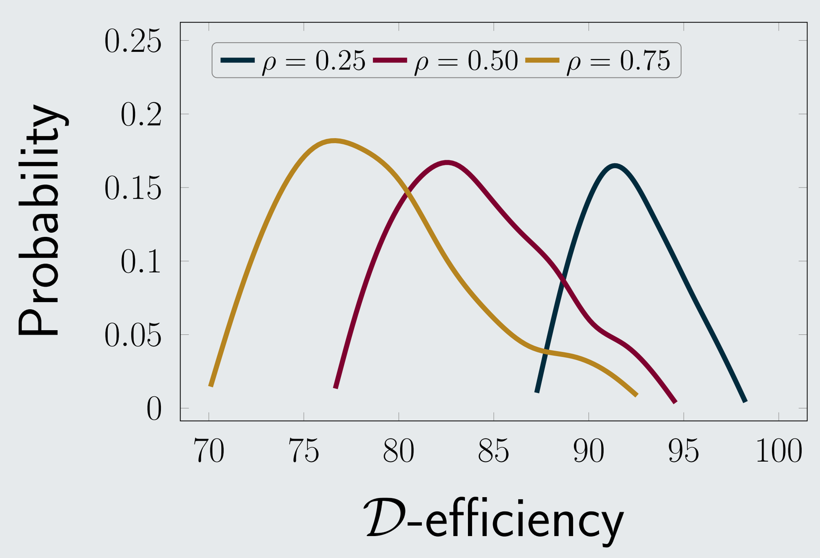
$\rho = 0$ $\qquad$ $\rho \neq 0$

Optimal designs for a split-plot experiment (with 1 hard-to-change factor) generated ignoring and considering autocorrelation

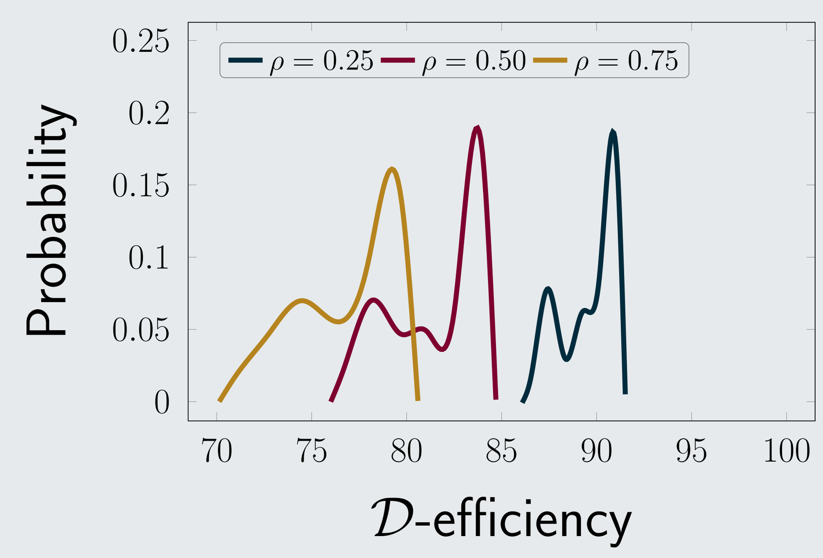
- **Designs generated ignoring autocorrelation** tend to have consecutive runs that share the same levels for some of the factors
- **Designs generated considering autocorrelation** tend to have consecutive runs with differing factor levels

Efficiency comparison of the optimal designs

- **When there is no autocorrelation:** the optimal designs generated considering autocorrelation are around 96% $\mathcal{D}$-efficient compared to the optimal designs generated ignoring autocorrelation
- **When there is autocorrelation:** it is likely that a random execution order for a blocked/split-plot design generated ignoring the autocorrelation, is substantially less $\mathcal{D}$-efficient than a design generated considering the autocorrelation, especially when ρ is large



Probability density function of the $\mathcal{D}$-efficiency of a blocked design generated ignoring the autocorrelation (compared to a design generated considering the autocorrelation)



Probability density function of the $\mathcal{D}$-efficiency of a split-plot design generated ignoring the autocorrelation (compared to a design generated considering the autocorrelation)

Influence of the value of ρ on the optimal designs when considering flexible numbers of blocks/whole plots with flexible sizes

$$\begin{array}{rrrr} \hline -1 & -1 & +1 & +1 \\ +1 & +1 & -1 & -1 \\ \hline +1 & +1 & -1 & -1 \\ -1 & -1 & +1 & +1 \\ \hline -1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 \\ \hline -1 & +1 & -1 & +1 \\ +1 & -1 & +1 & -1 \\ \hline +1 & -1 & -1 & +1 \\ -1 & +1 & +1 & -1 \\ \hline +1 & +1 & +1 & +1 \\ -1 & -1 & -1 & -1 \\ \hline \end{array} \qquad \begin{array}{rrrr} \hline -1 & +1 & +1 & +1 \\ +1 & -1 & -1 & -1 \\ -1 & +1 & +1 & +1 \\ \hline -1 & +1 & -1 & -1 \\ +1 & -1 & +1 & +1 \\ -1 & +1 & -1 & -1 \\ \hline -1 & -1 & -1 & +1 \\ +1 & +1 & +1 & -1 \\ -1 & -1 & -1 & +1 \\ \hline +1 & +1 & -1 & +1 \\ -1 & -1 & +1 & -1 \\ +1 & +1 & -1 & +1 \\ \hline \end{array}$$

$\rho = 0.25$ $\qquad$ $\rho = 0.75$

Optimal designs for a block experiment considering different values of ρ

$$\begin{array}{rrrr} \hline \mathbf{-1} & +1 & -1 & +1 \\ \mathbf{-1} & -1 & +1 & -1 \\ \hline \mathbf{-1} & -1 & +1 & -1 \\ \mathbf{-1} & +1 & -1 & +1 \\ \hline \mathbf{+1} & +1 & -1 & -1 \\ \mathbf{+1} & -1 & +1 & +1 \\ \hline \mathbf{+1} & -1 & -1 & -1 \\ \mathbf{+1} & +1 & +1 & +1 \\ \hline \mathbf{-1} & -1 & -1 & +1 \\ \mathbf{-1} & +1 & +1 & -1 \\ \hline \mathbf{+1} & +1 & +1 & -1 \\ \mathbf{+1} & -1 & -1 & +1 \\ \hline \end{array} \qquad \begin{array}{rrrr} \hline \mathbf{+1} & -1 & +1 & +1 \\ \mathbf{+1} & +1 & -1 & -1 \\ \mathbf{+1} & -1 & +1 & +1 \\ \hline \mathbf{+1} & +1 & +1 & -1 \\ \mathbf{+1} & -1 & -1 & +1 \\ \mathbf{+1} & +1 & +1 & -1 \\ \hline \mathbf{-1} & -1 & -1 & -1 \\ \mathbf{-1} & +1 & +1 & +1 \\ \mathbf{-1} & -1 & -1 & -1 \\ \hline \mathbf{+1} & +1 & -1 & +1 \\ \mathbf{+1} & -1 & +1 & -1 \\ \mathbf{+1} & +1 & -1 & +1 \\ \hline \end{array}$$

$\rho = 0.25$ $\qquad$ $\rho = 0.75$

Optimal designs for a split-plot experiment considering different values of ρ

- Different values of ρ lead to optimal designs with different grouping configurations