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

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## Linear mixed-effects model

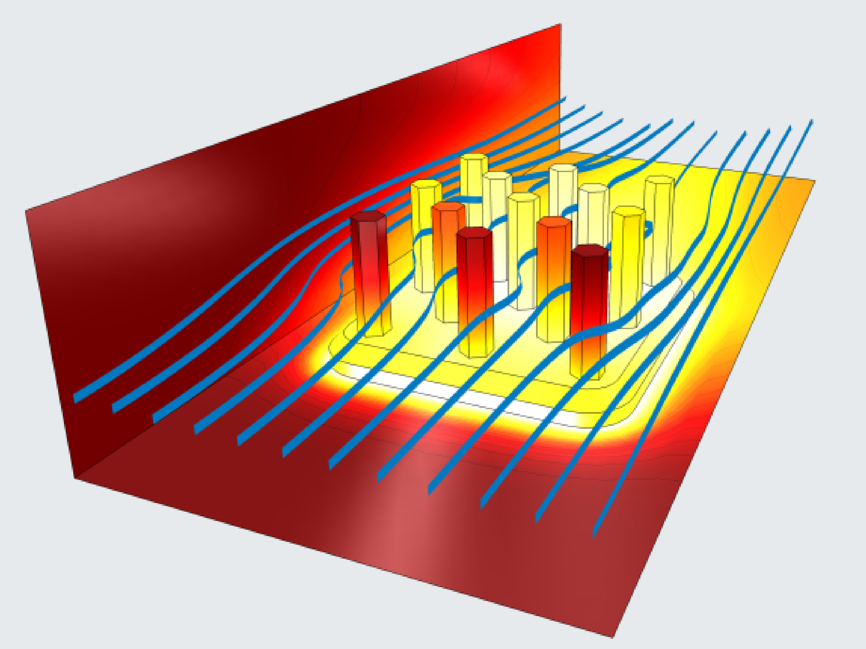
The model for analyzing a blocked/split-plot experiment involving $N$ runs, $F$ factors and $K$ blocks/whole plots is a mixed-effects model of the form

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

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 $N(0, \sigma_\delta^2)$)
- $\boldsymbol{\varepsilon}$ is the $N \times 1$ vector containing the residual errors of each observation (which follow a normal distribution $N(0, \sigma_\varepsilon^2)$)

## 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:

- $\eta$ is the variance ratio $\sigma_\delta^2/\sigma_\varepsilon^2$ that measures the extent to which observations in the same block/whole plot are correlated
- $\rho$ 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 $\rho$ and $\eta$

## Optimal designs generated ignoring and considering autocorrelation

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

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

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

Optimal designs for a block experiment generated ignoring and considering autocorrelation

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

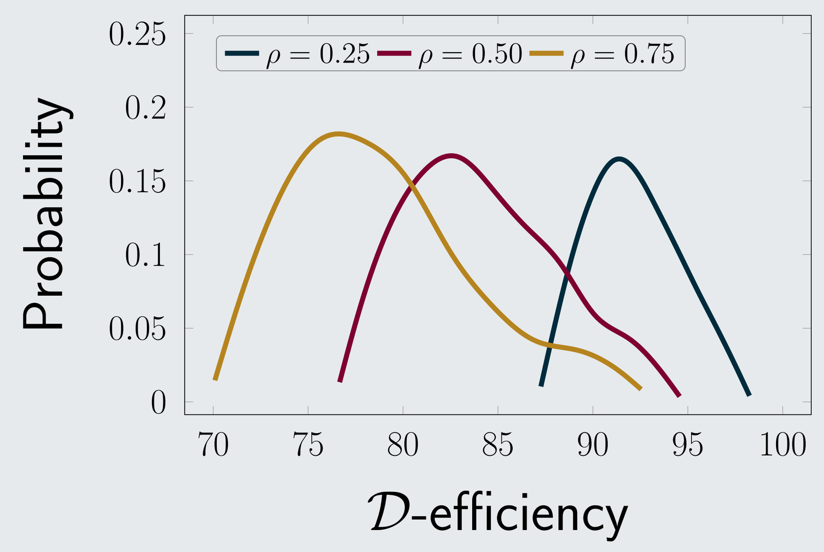
$\rho = 0$ $\qquad$ $\rho \neq 0$

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

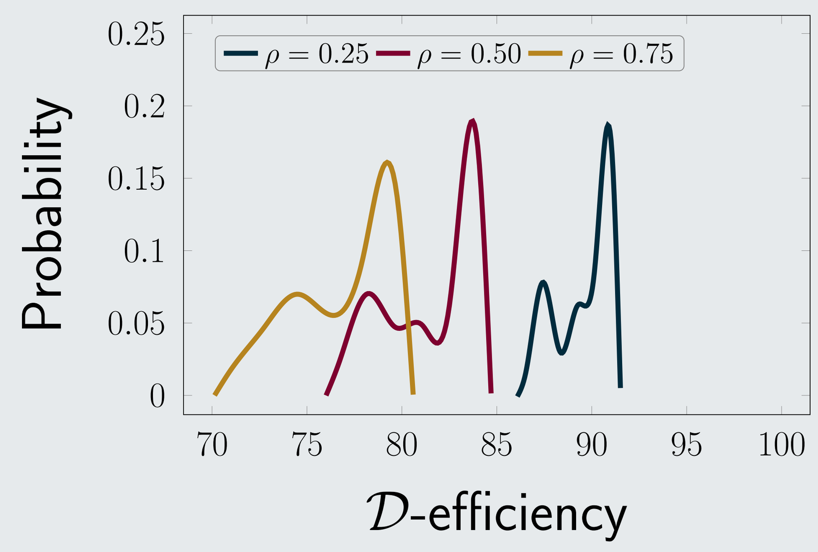
- **Designs generated ignoring autocorrelation** tend to have consecutive runs that share the same levels for some of the factors
- **Designs generated considering autocorrelation** tend to have consecutive runs with differing factor levels

## 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 $\rho$ 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 $\rho$ on the optimal designs when considering flexible numbers of blocks/whole plots with flexible sizes

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

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

Optimal designs for a block experiment considering different values of $\rho$

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

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

Optimal designs for a split-plot experiment considering different values of $\rho$

- Different values of $\rho$ lead to optimal designs with different grouping configurations