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Efficiencies of designs in the simple linear regression model with correlated errors

Model and problem

Point of departure: We consider designs ξ with n experimental units. Each unit consists of q design points $(x_1, \ldots, x_q)$. They are the same for all units.

Model for $n = 1$:

$$y = X_\xi \beta + e$$

with $y = \begin{bmatrix} y_1 \\ \vdots \\ y_q \end{bmatrix}$, $X_\xi = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_q \end{bmatrix}$, $\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$, $e = \begin{bmatrix} e_1 \\ \vdots \\ e_q \end{bmatrix}$. The vector e is normally distributed with $E(e) = 0$ and $Cov(e) = \Sigma(\sigma^2, \lambda)$.

Here $\Sigma(\sigma^2, \lambda) = \sigma^2 \begin{bmatrix} 1 & \lambda^{|x_2 - x_1|} & \ldots & \lambda^{|x_q - x_1|} \\ & 1 & & \vdots \\ & & \ddots & \lambda^{|x_q - x_{q-1}|} \\ & & & 1 \end{bmatrix}$ with $\lambda \in [0, 1]$.

$\rightarrow$ Correlations depend on the distances of the corresponding design points.

Model for $n \geq 1$:

$y = [y_{11}, \ldots, y_{1q}, y_{21}, \ldots, y_{nq}]^T$, $Cov(e) = I_n \otimes \Sigma(\sigma^2, \lambda) =: W$, design matrix: $1_n \otimes X_\xi =: \widetilde{X}$. Errors within one unit are correlated. Errors between different units are independent.

Parameters β_0 (intercept) and β_1 (slope) are of main interest, σ^2 (error variance) and λ (correlation parameter) are nuisance parameters.

D-criterion and D-efficiency:

$D(\xi) = (\det(\mathcal{I}_\xi^{-1}))^{\frac{1}{k}}$ with information matrix $\mathcal{I}_\xi$.

$eff_D(\xi) = \dfrac{D(\xi^*)}{D(\xi)}$, in which design ξ^* is D-optimal.

In what follows

- $q = 3$, $x_j \in [0, 1]$. $x_1 = 0$ and $x_3 = 1$, because the D-optimal designs observe at 0 and 1 (see [1]).
- How to choose $x_2 =: d$?

Nuisance parameters are known

Results in Dette et al. (2008):

- d and $1 - d$ lead to the same D-criterion.
- For $\lambda \rightarrow 1$: $d = 1/2$ is D-optimal.
- For $\lambda \in [0, 1)$: only locally D-optimal designs exist, see Figure 1.

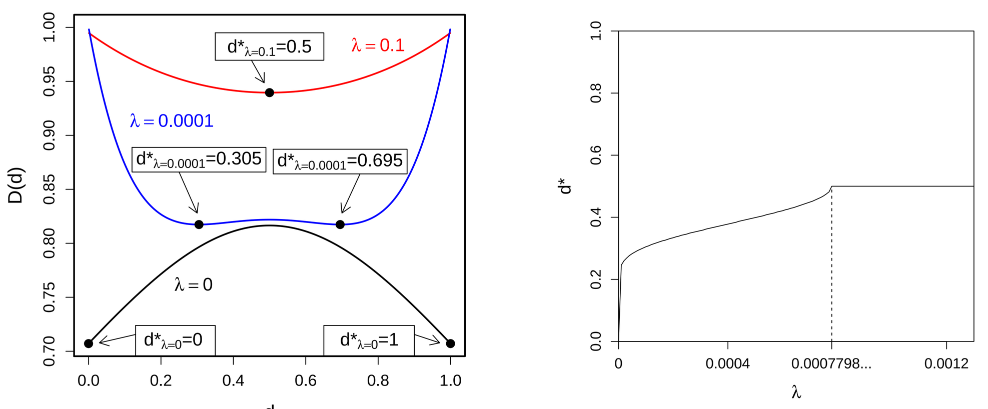

Figure 1: Left: D-criterion for selected correlations. Right: Locally D-optimal designs are presented.

New results:

- $d \in [0, 1]$:
  1. $d \in [0, 1]$: $eff_D(d) \geq 0.7071$ ($\lambda \in [0, 1]$).
  2. $d \in [0, 1]$: $eff_D(d) \geq 0.9$ ($\lambda \in [0.2, 1]$).
  3. $d \in [0, 1]$: $\lim_{\lambda \rightarrow 1} eff_D(d) = 1$.
  4. $d = 0$: min $eff_D(0) = 0.7071$.
  5. $d = 0.5$: $eff_D(0.5) \geq 0.8$ ($\lambda \in [0, 1)$).
- $d \in \{i/8 : 0, 1, \ldots, 8\}$:
  1. $d = 0$: min $eff_D(d) = 0.7493$.
  2. $d = 1/8$: min $eff_D(d) \geq 0.9220$.
  3. $d = 1/4$: min $eff_D(d) = 0.9014$.
  4. $d = 3/8$: min $eff_D(d) = 0.8750$.
  5. $d = 1/2$: min $eff_D(d) = 0.8660$.

Nuisance parameters are unknown

Two-step maximum likelihood estimation:

Likelihood function:

$$L_y(\beta, \sigma^2, \lambda) = \frac{1}{(2\pi)^{3n/2} \det(W)^{1/2}} \exp(-\frac{1}{2}(y - \widetilde{X}\beta)^T W^{-1} (y - \widetilde{X}\beta))$$

- **Step 1:**

(1) Determine $\hat{\beta}_{GLS}$ with $\lambda = 0$. Determine residuals $\hat{e}$.

(2) Replace $y - \widetilde{X}\beta$ with $\hat{e} \Longrightarrow L_y(\sigma^2, \lambda)$. Determine $\hat{\sigma}^2$ and $\hat{\lambda}$ by ML-estimators.

- **Step 2:**

(3) Determine $\hat{\beta}_{GLS}$ with $\hat{\lambda}$ out of (2). Determine residuals $\hat{e}$.

- **Repetition of two-step procedure:**

(4) Repeat (2) and (3) until estimates converge. Thereby use in (2) residuals of (3) instead of (1).

Oberhofer and Kmenta (1974): Estimates converge.

Simulation study:

$n \in \{2, 50\}$, $\lambda \in \{0, 0.1^4, 0.1^3, 0.1^2, 0.1, 0.25, 0.5, 0.9\}$,
$d \in \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6\}$, 10000 datasets for all combinations.

Results:

First line: empirical D-criterion (blue = locally D-optimal design (empirical))
Second line: theoretical D-criterion (red = locally D-optimal design (nuisance parameters are known))

	$n = 2$						$n = 50$					
	d						d					
λ	0.1	0.2	0.3	0.4	0.5	0.6	0.1	0.2	0.3	0.4	0.5	0.6
0	0.731	0.760	0.796	0.806	0.811	0.817	0.735	0.769	0.802	0.799	0.823	0.802
	0.742	0.771	0.796	0.811	0.817	0.811	0.742	0.771	0.796	0.811	0.817	0.811
0.0001	0.863	0.832	0.830	0.825	0.814	0.831	0.886	0.817	0.817	0.828	0.821	0.826
	0.873	0.827	0.817	0.820	0.822	0.820	0.873	0.827	0.817	0.820	0.822	0.820
0.001	0.914	0.858	0.842	0.842	0.842	0.835	0.896	0.850	0.841	0.841	0.831	0.841
	0.903	0.857	0.838	0.834	0.833	0.834	0.903	0.857	0.838	0.834	0.833	0.834
0.01	0.940	0.915	0.880	0.879	0.868	0.857	0.931	0.903	0.888	0.869	0.879	0.860
	0.939	0.901	0.880	0.869	0.867	0.869	0.939	0.901	0.880	0.869	0.867	0.869
0.1	0.979	0.980	0.953	0.954	0.940	0.943	0.965	0.960	0.940	0.943	0.948	0.938
	0.974	0.958	0.948	0.942	0.940	0.942	0.974	0.958	0.948	0.942	0.940	0.942
0.25	0.975	0.949	0.948	0.943	0.954	0.958	0.954	0.972	0.943	0.953	0.950	0.943
	0.961	0.956	0.952	0.949	0.949	0.949	0.961	0.956	0.952	0.949	0.949	0.949
0.5	0.871	0.883	0.867	0.867	0.843	0.863	0.857	0.865	0.868	0.864	0.869	0.862
	0.865	0.864	0.863	0.863	0.863	0.863	0.865	0.864	0.863	0.863	0.863	0.863
0.9	0.439	0.439	0.439	0.432	0.439	0.434	0.434	0.438	0.435	0.439	0.434	0.435
	0.436	0.436	0.436	0.436	0.436	0.436	0.436	0.436	0.436	0.436	0.436	0.436

- Empirical D-criterion is close to the theoretical D-criterion.
- Only locally D-optimal designs exist.
- Results for known nuisance parameters can be transferred to the case of unknown parameters even if the number of experimental units is small.

References

[1] Dette, H., Kunert, J. and Pepelyshev, A. (2008). Exact optimal designs for weighted least squares analysis with correlated errors. *Statistica Sinica* **18**, 135-154.

[2] Oberhofer, W. and Kmenta, J. (1974). A general procedure for obtaining maximum likelihood estimates in generalized regression models. *Econometrika* **42**, 579-590.

SFB 823
Statistical modelling of nonlinear dynamic processes