Optimal design for linear models with correlated observations

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Outline

1. Linear models with correlated observations
   - Least squares versus weighted least squares estimation
   - Approximate (continuous) designs
   - Admissible designs

2. Optimal designs
   - Necessary condition
   - $D$- and $c$-optimality

3. Universally optimal designs
   - Integral operators
   - Necessary and sufficient conditions for universal optimality
   - Proof (ideas)

4. Examples

5. $g$-optimal designs
Linear regression model

- Common linear regression model

\[ y(x) = \theta_1 f_1(x) + \ldots + \theta_m f_m(x) + \varepsilon(x), \]

- \( f_1, \ldots, f_m \) are linearly independent, continuous (regression) functions
- \( \theta_1, \ldots, \theta_m \) are unknown parameters
- \( N \) observations

\[ y_1 = y(x_1), \ldots, y_N = y(x_N) \]

at experimental conditions \( x_1, \ldots, x_N \in \mathcal{X} \subset \mathbb{R}^d \)
Correlation

- Correlation structure

  \[
  E[\varepsilon(x_i)] = 0, \quad E[\varepsilon(x_i)\varepsilon(x_j)] = K(x_i, x_j); \quad x_i, x_j \in \mathcal{X}
  \]

- Here \( K \) is a kernel representing the covariance structure, which satisfies
  
  - positive definite
  
  - \( K(u, v) \neq 0 \) for all \((u, v) \in \mathcal{X} \times \mathcal{X}\)
  
  - continuous at all points \((u, v) \in \mathcal{X} \times \mathcal{X}\) except possibly at the diagonal points \((u, u)\)

- **Design problem**: optimal allocation of \( x_1, \ldots, x_N \) for most efficient estimation of \( \theta_1, \ldots, \theta_m \)
Estimation

- Least squares estimation (LSE)
  \[ \hat{\theta} = (X^T X)^{-1} X^T Y \]

  where
  - \( X = (f_i(x_j))_{j=1,\ldots,N} \)
  - \( Y = (y_1, \ldots, y_N)^T \)

- Covariance matrix of \( \hat{\theta} \)
  \[ \text{Var}(\hat{\theta}) = (X^T X)^{-1} X^T \Sigma X (X^T X)^{-1} \]

  where
  \[ \Sigma = (K(x_i, x_j))_{i,j=1,\ldots,N} \]
Weighted versus unweighted least squares

- Weighted least squares estimation (BLUE)
  \[ \hat{\theta} = (X^T \Sigma^{-1} X)^{-1} X^T \Sigma^{-1} Y \]

- Covariance matrix of \( \hat{\theta} \)
  \[ \text{Var}(\hat{\theta}) = (X^T \Sigma^{-1} X)^{-1} \leq \text{Var}(\tilde{\theta}) \]

  where
  \[ \Sigma = (K(x_i, x_j))_{i,j=1,...,N} \]

- **Note:** We focus on ordinary least squares estimation (LSE)
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- **Note:** We focus on ordinary least squares estimation (LSE)
Weighted versus unweighted least squares

**Note:** We focus on ordinary least squares estimation (LSE) because

1. BLUE is often sensitive with respect to misspecification of $\Sigma$ (LSE is more robust)
2. The difference between BLUE and LSE is often surprisingly small [Rao (1967), Kruskal (1968)]
3. We will give a heuristic explanation of this phenomenon and will additionally derive conditions such that

$$LSE + \text{optimal design} = BLUE + \text{optimal design}$$
Motivation (one dimensional case)

- $a : \mathcal{X} \rightarrow [0, 1]$ distribution function on $\mathcal{X} \subset \mathbb{R}$
- Design points are quantiles of $a$, that is
  \[ x_i = a^{-1}((i - 1)/(N - 1)), \quad i = 1, \ldots, N, \]

- If $\xi_N$ is the probability measure with masses $1/N$ at $x_i$, then
  \[ \text{Var}(\tilde{\theta}) = D(\xi_N) = M^{-1}(\xi_N)B(\xi_N, \xi_N)M^{-1}(\xi_N) \]
  where
  \[ M(\xi_N) = \int_{\mathcal{X}} f(u)f^T(u)\xi_N(du) \]
  \[ B(\xi_N, \xi_N) = \iint K(u, v)f(u)f^T(v)\xi_N(du)\xi_N(dv) \]
  and $f = (f_1, \ldots, f_m)^T$ is the vector of regression functions.
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Approximate (continuous) designs

For a probability measure $\xi$ on $\mathcal{X}$ (more precisely on its Borel field) the matrix

$$D(\xi) = M^{-1}(\xi)B(\xi, \xi)M^{-1}(\xi)$$

is called the **information matrix** (for LSE) of the design $\xi$, where

- $M(\xi) = \int_{\mathcal{X}} f(u)f^T(u)\xi(du)$
- $B(\xi, \xi) = \int\int K(u, v)f(u)f^T(v)\xi(du)\xi(dv)$
Admissible designs

Define

\[ \mathcal{X}_1 = \mathcal{X} \setminus \mathcal{X}_0 = \{ x \in \mathcal{X} : f(x) \neq 0 \} \]

Assume that designs \( \xi_0 \) and \( \xi_1 \) are concentrated on \( \mathcal{X}_0 \) and \( \mathcal{X}_1 \) correspondingly.

The design \( \xi_\alpha = \alpha \xi_0 + (1 - \alpha) \xi_1 \) satisfies

\[
D(\xi_\alpha) = M^{-1}(\xi_\alpha) B(\xi_\alpha, \xi_\alpha) M^{-1}(\xi_\alpha) = D(\xi_1)
\]

(for all \( 0 \leq \alpha < 1 \))

For the theoretical part of this talk we assume \( f(x) \neq 0 \) for all \( x \in \mathcal{X} \)
Admissible designs

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- For the theoretical part of this talk we assume \( f(x) \neq 0 \) for all \( x \in X \)
Optimal design

- Let $\Phi(\cdot)$ be a monotone, convex real valued functional defined on the space of symmetric $m \times m$ matrices.

- The design $\xi$ is $\Phi$-optimal, if it minimizes the function

$$\Phi(D(\xi)) = \Phi(M^{-1}(\xi)B(\xi, \xi)M^{-1}(\xi))$$

among all designs on the design space $\mathcal{X}$, where

- $M(\xi) = \int_{\mathcal{X}} f(u)f^T(u)\xi(du)$

- $B(\xi, \xi) = \int \int K(u, v)f(u)f^T(v)\xi(du)\xi(dv)$

A further definition:

$$B(\xi, \nu) = \int_{\mathcal{X}} \int_{\mathcal{X}} K(u, v)f(u)f^T(v)\xi(du)\nu(dv),$$
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\]
A necessary condition

**Theorem**

*If the matrix of derivatives*

\[ C = \frac{\partial \Phi(D)}{\partial D} = \left( \frac{\partial \Phi(D)}{\partial D_{ij}} \right)_{i,j=1,\ldots,m} \]

*exists and \( \xi^* \) minimizes \( \Phi(D(\xi)) \), then the inequality*

\[
 f^T(x)D(\xi^*)C(\xi^*)M^{-1}(\xi^*)f(x) \leq \text{tr}(C(\xi^*)M^{-1}(\xi^*)B(\xi^*, \xi_x)M^{-1}(\xi^*)) \tag{1}
\]

*holds for all \( x \in \mathcal{X} \), where*

\[
 B(\xi^*, \xi_x) = \int_{\mathcal{X}} K(u, x)f(u)\xi^*(du)f^T(x).
\]

*Moreover, there is equality in (1) for \( \xi^* \)-almost all \( x \)*
Linear models with correlated observations
Optimal designs
Universally optimal designs
Examples
\(g\)-optimal designs

\(D\)- and \(c\)-optimality

Two examples:

- The necessary condition is of the form
  \[
  d(x, \xi^*) \leq b(x, \xi^*) \quad \text{for all} \quad x \in \mathcal{X}
  \]

- \(D\)-optimality; \(\Phi(D(\xi)) = -\log \det(D(\xi))\)

  \[
  f^T(x)M^{-1}(\xi^*)f(x) \leq f^T(x)B^{-1}(\xi^*, \xi^*) \int K(u, x)f(u)\xi^*(du)
  \]

- \(c\)-optimality (for a given \(c \in \mathbb{R}^m\)); \(\Phi(D(\xi)) = c^TD(\xi)c\)

  \[
  f^T(x)M^{-1}(\xi^*)cc^TM^{-1}(\xi^*)
  \times \left( \int K(x, u)f(u)\xi^*(du) - B(\xi^*, \xi^*)M^{-1}(\xi^*)f(x) \right) \geq 0
  \]
**Figure:** The functions $b(x, \xi)$ and $d(x, \xi)$ in the necessary condition

$$d(x, \xi^*) \leq b(x, \xi^*)$$

for the covariance kernels $K(u, v) = e^{-|u-v|}$, $K(u, v) = -\log((u - v)^2)$ and $K(u, v) = \max(0, 1 - |u - v|)$. $\xi^*$ is arcsine design, i.e.

$$\frac{d\xi^*}{dx} = \frac{1}{\pi \sqrt{1 - x^2}}$$
Comments: the lack of convexity

- **Note:** The conditions are "only" necessary. This means:
  
  - The arcsine design is **not** $D$-optimal for quadratic regression with a covariance kernel
    
    $$K(u, v) = e^{-|u-v|} \quad \text{or} \quad K(u, v) = \max(0, 1 - |u-v|)$$
  
  - For the logarithmic kernel
    
    $$K(u, v) = -\log(u - v)^2$$
    
    we observe equality in the necessary condition for all $x$.
  
  → The arcsine design **might** be $D$-optimal for quadratic regression with logarithmic kernel
Comments: the lack of convexity

- Optimality results are only available for the location model
  \[ y(x) = \theta + \varepsilon(x) \]
  (in this case the criterion is fact convex).

- In the following discussion we propose a method for deriving
  optimality results for more general models:
  - regression models with more than one regression function and
    an associated covariance kernel
  - universally optimal designs
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In the following discussion we propose a method for deriving optimality results for more general models:

- regression models with more than one regression function and an associated covariance kernel
- universally optimal designs
Universally optimal designs

- A design $\xi^*$ is **universally** optimal if and only if

  $$D(\xi^*) \leq D(\xi)$$

  in the sense of the Loewner ordering for any design $\xi \in \Xi$, that is

  $$c^T D(\xi^*) c \leq c^T D(\xi) c$$

  for all $c \in \mathbb{R}^m$.

- A design $\xi^*$ is universally optimal if and only if it is $c$-optimal for all $c \in \mathbb{R}^m$. 

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A design $\xi^*$ is universally optimal if and only if it is $c$-optimal for all $c \in \mathbb{R}^m$. 
A crucial representation

- For any design $\xi$ we have the representation

$$\int K(x, u)f(u)\xi(du) = \Lambda f(x) + g_\xi(x), \quad x \in \mathcal{X},$$

where $\Lambda = B(\xi, \xi)M^{-1}(\xi)$ and the function $g_\xi$ satisfies.

$$\int g_\xi(x)f^T(x)\xi(dx) = 0$$

Note:

- The function $g_\xi$ depends on the design $\xi$ and the kernel $K$.
- If $g_\xi \equiv 0$ and $\Lambda$ is diagonal, then the regression functions $f = (f_1, \ldots, f_m)^T$ are eigenfunctions of the integral operator associated with the kernel $K$ and the design $\xi$. 
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Theorem

Consider the linear regression model with a covariance kernel $K$, a design $\xi \in \Xi$ and the corresponding the vector-function $g_\xi(\cdot)$ defined by

$$g_\xi(x) = \int K(x, u)f(u)\xi(du) - \Lambda f(x), \quad x \in X,$$

If $g_\xi(x) = 0$ for all $x \in X$, then the design $\xi$ is universally optimal.
Proof (first idea)

- Check $c$-optimality for any $c \in \mathbb{R}^m$
- Necessary condition:

$$f^T(x)M^{-1}(\xi)cc^T M^{-1}(\xi)\left(\int K(x, u)f(u)\xi(du) - B(\xi, \xi)M^{-1}(\xi)f(x)\right) \geq 0$$

$$g_\xi(x) \equiv 0$$

- $\xi$ is a candidate for universal optimality!
- However, the criterion is not convex!
Proof (idea)

- **Idea of a rigorous proof:** simultaneous optimal estimation and optimization of the design in the model

\[ y(x) = \theta^T f(x) + \varepsilon(x) \]

where the full trajectory \( \{y(x)|x \in \mathcal{X}\} \) can be observed.

- **Arbitrary (linear) estimate:** if \( \mu = (\mu_1, \ldots, \mu_m)^T \) is a vector of signed measures

\[
\hat{\theta}(\mu) = \int y(x) \mu(dx)
\]

- Unbiasedness means here

\[
\int \mu(dx)f^T(x) = \int f(x)\mu^T(dx) = I_m,
\]

- E.g. \( \mu_\xi(dx) = M^{-1}(\xi)f(x)\xi(dx) \) gives LSE for the design \( \xi \)
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Proof (idea)

- **Note:** The variance of $c^T \hat{\theta}(\mu)$ is given by

$$\text{Var}(c^T \hat{\theta}(\mu)) = c^T \int \int \mathbb{E}[\varepsilon(x)\varepsilon(u)] \mu(dx) \mu^T(du)c$$

$$= c^T \int \int K(x,u) \mu(dx) \mu^T(du)c =: \Phi_c(\mu)$$

- This function is convex with respect to $\mu$!
Proof (idea)

- Standard equivalence theory (convex optimization) is applicable!

- A vector of signed measures $\mu^*$ minimizes

$$\Phi_c(\mu) = c^T \int \int K(x, u) \mu(dx) \mu^T(du)c$$

if and only if the inequality

$$c^T \int \int K(x, u) \mu^*(dx) \nu^T(du)c \geq \Phi_c(\mu^*)$$

holds for all vector valued signed measures $\nu$ corresponding to unbiased estimates.
Proof (idea)

- We use
  \[ \mu^*(dx) = M^{-1}(\xi)f(x)\xi(dx), \]  
  which yields an unbiased estimator
- Note that \((g_\xi \equiv 0, \text{by assumption of the Theorem})\)
  \[ \int K(x, u)f(x)\xi^*(dx) = \Lambda f(u) \]  

Left hand side of equivalence theorem

\[ c^T \int \int K(x, u)\mu^*(dx)\nu^T(du)c \]
\[ \overset{2}{=} c^T M^{-1}(\xi) \int \int K(x, u)f(x)\xi(dx)\nu^T(du)c \]
\[ \overset{3}{=} c^T M^{-1}(\xi) \int \Lambda f(u)\nu^T(du)c \overset{unbiased}{=} c^T M^{-1}(\xi)\Lambda c \]
Proof (idea)

- We use
  \[ \mu^*(dx) = M^{-1}(\xi)f(x)\xi(dx), \quad (2) \]
  which yields an unbiased estimator
- Note that \( g\xi \equiv 0 \), by assumption of the Theorem)
  \[ \int K(x, u)f(x)\xi^*(dx) = \Lambda f(u) \quad (3) \]
- Left hand side of equivalence theorem
  \[
  c^T \int \int K(x, u)\mu^*(dx)\nu^T(du)c \\
  \overset{(2)}{=} c^T M^{-1}(\xi) \int \int K(x, u)f(x)\xi(dx)\nu^T(du)c \\
  \overset{(3)}{=} c^T M^{-1}(\xi) \int \Lambda f(u)\nu^T(du)c \overset{\text{unbiased}}{=} c^T M^{-1}(\xi)\Lambda c \]
We use
\[ \mu^*(dx) = M^{-1}(\xi^*) f(x)\xi^*(dx), \]  
(4)

Right hand side of equivalence theorem (with similar arguments)
\[ \Phi_c(\mu^*) = c^T M^{-1}(\xi) \Lambda c \]
\[ = c^T M^{-1}(\xi) B(\xi, \xi) M^{-1}(\xi) c = D(\xi) \]

\( \mu^* \) minimizes \( \Phi_c \) in the class of all vector valued signed measures corresponding to unbiased estimates!
Proof (idea)

- Now return to the minimization of \( D(\eta) \) in the class of all designs \( \eta \in \Xi \).
- For any \( \eta \in \Xi \) consider the corresponding vector-valued signed measure \( \mu_\eta(dx) = M^{-1}(\eta)f(x)\eta(dx) \), then

\[
    c^T D(\eta) c = c^T M^{-1}(\eta)B(\eta, \eta)M^{-1}(\eta)c = \Phi_c(\mu_\eta) \\
    \geq \min_{\mu} \Phi_c(\mu) = \Phi_c(\mu^*) = c^T D(\xi)c.
\]

- Since the design \( \xi \) does not depend on the particular vector \( c \), it follows that \( \xi \) is universally optimal.
**Theorem**

Consider the linear regression model with a covariance kernel $K$, a design $\xi \in \Xi$ and the corresponding function $g_\xi(\cdot)$ defined by

$$g_\xi(x) = \int K(x, u)f(u)\xi(du) - \Lambda f(x), \quad x \in \mathcal{X},$$

If the design $\xi$ is universally optimal, then the function $g_\xi(\cdot)$ can be represented in the form

$$g_\xi(x) = \gamma(x)f(x),$$

where $\gamma(x)$ is a non-negative function such that $\gamma(x) = 0$ for all $x$ in the support of the design $\xi$. 

$g_\xi \equiv 0$ is ”necessary” for universal optimality.
Remarks:

- **Note:** If $g_\xi \equiv 0$ then LSE with the optimal design can **not** be improved by any BLUE!

\[ \text{LSE + optimal design} = \text{BLUE + optimal design} \]

- Mercer’s theorem provides numerous models for which universally optimal designs can be identified explicitly [see e.g. Kanwal (1997)]
Remarks:

- Integral operator on $L_2(\xi)$

$$T_K(f)(\cdot) = \int_X K(\cdot, u)f(u)\xi(du)$$

Under certain assumptions on the kernel $T_K$ defines a symmetric, compact self-adjoint operator.

- Mercer’s theorem: there exist a countable number of eigenfunctions

$$\varphi_1, \varphi_2, \ldots$$

with positive eigenvalues

$$\lambda_1, \lambda_2, \ldots$$

of the operator $K$
Theorem

- Assume that the covariance kernel \( K(x, u) \) defines an integral operator \( T_K \) with corresponding eigenfunctions \( \varphi_1, \varphi_2, \ldots \).

- For any non-singular matrix \( L \in \mathbb{R}^{m \times m} \) consider the linear regression model

\[
\theta^T f(x) = \theta^T L(\varphi_{i_1}(x), \ldots, \varphi_{i_m}(x))^T
\]

with covariance kernel \( K(x, u) \).

- Then the design \( \xi \) is universally optimal!
Consider the regression functions

\[ f_j(x) = \begin{cases} 
  1 & \text{if } j = 1 \\
  \sqrt{2} \cos(2\pi(j - 1)x) & \text{if } j \geq 2 
\end{cases} \]  

(5)

on the design space \( \mathcal{X} = [0, 1] \).

**Note:** Linear models with regression functions (5) are widely applied in series estimation in nonparametric regression [see e.g. Efromovich (1999), Tsybakov (2009)].

If \( K(x, y) = \rho(x - y) \) (stationarity) where \( \rho \) is periodic with period 1
\[ \rightarrow \text{the uniform design is universally optimal!} \]
Example: polynomial regression

- Consider the regression functions

\[ f_j(x) = x^{j-1}, \ j = 1, \ldots, m + 1 \quad (6) \]

on the design space \( X = [-1, 1] \).

- If \( K(x, y) = -\log |x - y| \) (stationarity)

\[ \rightarrow \text{the arcsine design is universally optimal!} \]

\[ \frac{d\xi^*}{dx} = \frac{1}{\pi \sqrt{1 - x^2}} \]
Example: spherical descriptors

- For $n = 0, 1, \ldots ; m = -n, -n + 2, \ldots, n - 2, n$ define

$$Y^m_n(\varphi, \phi) = \sqrt{\frac{2n + 1}{4\pi}} \frac{n - |m|}{n + |m|} P^{|m|}_n(\cos \varphi \exp(im\psi))$$

where $\varphi \in [0, \pi], \psi \in [0, 2\pi]$,

$$P^m_n(x) = (-1)^m (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_n(x)$$

and $P_n$ is the $n$th Legendre polynomial.

- The uniform distribution on $[0, \pi] \times [0, 2\pi]$ is universally optimal for the kernels

$$K(u, v) = \exp(-\|u - v\|^2), \quad K(u, v) = (1 + \langle u, v \rangle)^d \quad (d \in \mathbb{N})$$
Future research: $g$-Optimal Designs

- **Recall:** the condition
  \[ g_\xi(x) = \int_X K(x, u)f(u)\xi(du) - B(\xi, \xi)M^{-1}(\xi)f(x) \equiv 0 \]
  is "necessary and sufficient" for universal optimality

- A **$g$-optimal design** minimizes
  \[ \|g_\xi\|_2^2 = \int_X |g_\xi(x)|^2 d\xi(x) \]

- **Note:** This criterion seeks for designs "close" to universal optimality

- A multiplicative algorithm is available, which yields $g$-optimal designs.

- We expect that these designs have "good" with respect to many optimality criteria
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**g-optimal designs for quadratic regression**

- Quadratic regression model with correlation function
  \[ K(x, y) = \exp(-\lambda|x - y|) \]
- \( \mathcal{X} = [-1, 1] \)
- \( g \)-optimal designs for \( \lambda = 1 \) (left), \( \lambda = 4 \) (middle) and \( \lambda = 8 \) (right).
**g-optimal designs for quadratic regression**

- Quadratic regression model with correlation function
  \[ K(x, y) = \exp(-\lambda|x - y|) \]
- \[ \mathcal{X} = [-1, 1] \]
- \( D-, A \)-efficiency of the \( g \)-optimal and uniform design.

| \( \xi \)     | \( \lambda = 1 \) | \( \lambda = 4 \) | \( \lambda = 8 \) |
|----------------|-----------------|-----------------|-----------------|
| \( \xi_g \)   | \( \text{Eff}_D(\xi) \) | \( \text{Eff}_A(\xi) \) | \( \text{Eff}_D(\xi) \) | \( \text{Eff}_A(\xi) \) |
| \( \xi_u \)   | \( 0.996 \)    | \( 0.993 \)    | \( 0.998 \)    | \( 0.996 \)    |
|                | \( 0.821 \)    | \( 0.832 \)    | \( 0.851 \)    | \( 0.822 \)    |
|                | \( 0.999 \)    | \( 0.998 \)    | \( 0.999 \)    | \( 0.998 \)    |
|                | \( 0.910 \)    | \( 0.881 \)    | \( 0.910 \)    | \( 0.881 \)    |
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