Optimal design for linear models with correlated observations

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Nice, July 2013

Outline

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

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

- Here K is a kernel representing the covariance structure, which satisifies
  - 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)

$$\tilde{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

where

  - $\mathbf{X} = (f_i(x_j))_{j=1,\dots,N}^{i=1,\dots,m}$
  - $\mathbf{Y} = (y_1, \dots, y_N)^T$

- Covariance matrix of $\tilde{\theta}$

$$\mathrm{Var}(\tilde{\theta}) = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{\Sigma}\mathbf{X}\,(\mathbf{X}^T\mathbf{X})^{-1}$$

where

$$\mathbf{\Sigma} = (K(x_i, x_j))_{i,j=1,\dots,N}$$

Weighted versus unweighted least squares

- Weighted least squares estimation (BLUE)

$$\hat{\theta} = (\mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{Y}$$

- Covariance matrix of $\hat{\theta}$

$$\mathrm{Var}(\hat{\theta}) = (\mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{X})^{-1} \leq \mathrm{Var}(\tilde{\theta})$$

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$$\mathbf{\Sigma} = (K(x_i, x_j))_{i,j=1,\ldots,N}$$

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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 Σ (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)

- $a : \mathcal{X} \to [0, 1]$ distribution function on $\mathcal{X} \subset \mathbb{R}$
- Design points are quantiles of a, that is

$$x_i = a^{-1}((i-1)/(N-1)), \; i = 1, \dots, N,$$

- If ξ_N is the probability measure with masses $1/N$ at x_i, then

$$\mathrm{Var}(\tilde{\theta}) = D(\xi_N) = M^{-1}(\xi_N) B(\xi_N, \xi_N) M^{-1}(\xi_N)$$

where

- $M(\xi_N) = \int_{\mathcal{X}} f(u) f^T(u) \xi_N(\mathrm{d}u)$
- $B(\xi_N, \xi_N) = \int\int K(u, v) f(u) f^T(v) \xi_N(\mathrm{d}u) \xi_N(\mathrm{d}v)$

and $f = (f_1, \dots, f_m)^T$ is the vector of regression functions.

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Approximate (continuous) designs

- For a probability measure ξ 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 ξ, where

  - $M(\xi) = \int_{\mathcal{X}} f(u)f^T(u)\xi(\mathrm{d}u)$
  - $B(\xi,\xi) = \int\int K(u,v)f(u)f^T(v)\xi(\mathrm{d}u)\xi(\mathrm{d}v)$

Admissible designs

- Define

$$\mathcal{X}_1 = \mathcal{X} \backslash \mathcal{X}_0 = \{x \in \mathcal{X} : f(x) \neq 0\}$$

- Assume that designs ξ_0 and ξ_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 $x \in \mathcal{X}$

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Optimal design

- Let $\Phi(\cdot)$ be a monotone, convex real valued functional defined on the space of symmetric $m \times m$ matrices
- The design ξ is **Φ-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

  - $M(\xi) = \int_{\mathcal{X}} f(u)f^T(u)\xi(\mathrm{d}u)$
  - $B(\xi,\xi) = \int\int K(u,v)f(u)f^T(v)\xi(\mathrm{d}u)\xi(\mathrm{d}v)$

- A further definition:

$$B(\xi,\nu) = \int_{\mathcal{X}}\int_{\mathcal{X}} K(u,v)f(u)f^T(v)\xi(\mathrm{d}u)\nu(\mathrm{d}v),$$

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A necessary condition

Theorem

If the matrix of derivatives

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

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

$$f^T(x) D(\xi^*)\, C(\xi^*) M^{-1}(\xi^*) f(x) \;\le\; tr\big(C(\xi^*) M^{-1}(\xi^*) B(\xi^*, \xi_x) M^{-1}(\xi^*)\big) \qquad (1)$$

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

$$B(\xi^*, \xi_x) = \int_{\mathcal{X}} K(u, x) f(u) \xi^*(\mathrm{d}u) f^T(x).$$

Moreover, there is equality in (1) *for* ξ^**-almost all* x

Two examples:

- The necessary condition is of the form

$$d(x,\xi^*) \;\le\; b(x,\xi^*) \quad \text{for all} \quad x \in \mathcal{X}$$

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

$$f^T(x)M^{-1}(\xi^*)f(x) \;\le\; f^T(x)B^{-1}(\xi^*,\xi^*)\int K(u,x)f(u)\xi^*(\mathrm{d}u)$$

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

$$f^T(x)M^{-1}(\xi^*)cc^T M^{-1}(\xi^*) \times\Big(\int K(x,u)f(u)\xi^*(du) - B(\xi^*,\xi^*)M^{-1}(\xi^*)f(x)\Big) \;\ge 0$$

Quadratic regression on the interval $[-1, 1]$

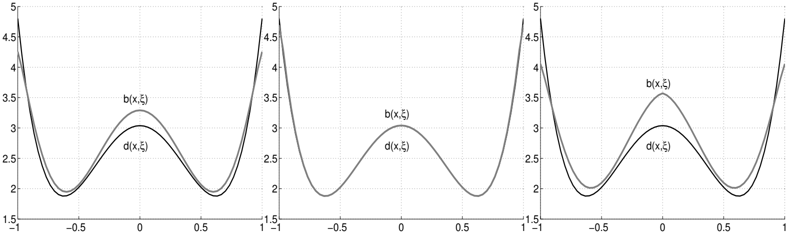

Figure: *The functions $b(x, \xi)$ and $d(x, \xi)$ in the necessary condition*

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

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

$$K(u,v) = e^{-|u-v|} \text{ or } K(u,v) = \max(0, 1-|u-v|)$$

  - For the logarithmic kernel

$$K(u,v) = -\log(u-v)^2$$

  we observe equality in the necessary condition for all x.

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

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A crucial representation

- For any design ξ 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_ξ satisfies.

$$\int g_\xi(x) f^T(x)\xi(\mathrm{d}x) = 0$$

- **Note:**
  - The function g_ξ depends on the design ξ and the kernel K
  - If $g_\xi \equiv 0$ and Λ 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 ξ

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$g_\xi \equiv 0$ is sufficient for universal optimality

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

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

If $g_\xi(x) = 0$ for all $x \in \mathcal{X}$, then the design ξ is universally optimal.

Proof (first idea)

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

$$f^T(x)M^{-1}(\xi)cc^TM^{-1}(\xi)\underbrace{\Big(\int K(x,u)f(u)\xi(du) - B(\xi,\xi)M^{-1}(\xi)f(x)\Big)}_{g_\xi(x)\equiv 0} \geq 0$$

- ξ 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**

$$\hat{\theta}(\mu) = \int y(x)\mu(\mathrm{d}x)$$

- Unbiasedness means here

$$\int \mu(\mathrm{d}x) f^T(x) = \int f(x)\mu^T(\mathrm{d}x) = I_m \,,$$

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

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Proof (idea)

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

$$\begin{aligned}\mathrm{Var}(c^T\hat{\theta}(\mu)) &= c^T\int\int \mathrm{E}[\varepsilon(x)\varepsilon(u)]\mu(dx)\mu^T(du)c \\ &= c^T\int\int K(x,u)\mu(\mathrm{d}x)\mu^T(\mathrm{d}u)c \;=:\; \Phi_c(\mu)\end{aligned}$$

- **This function is convex with respect to μ!**

Proof (idea)

- Standard equivalence theory (convex optimization) is applicable!

- A vector of signed measures μ^* minimizes

$$\Phi_c(\mu) = c^T \int \int K(x,u)\mu(\mathrm{d}x)\mu^T(\mathrm{d}u)c$$

if and only if the inequality

$$c^T \int \int K(x,u)\mu^*(\mathrm{d}x)\nu^T(\mathrm{d}u)c \geq \Phi_c(\mu^*)$$

holds for all vector valued signed measures ν corresponding to unbiased estimates.

Proof (idea)

- We use
$$\mu^*(\mathrm{d}x) = M^{-1}(\xi) f(x) \xi(\mathrm{d}x), \tag{2}$$
which yields an unbiased estimator
- Note that ($g_\xi \equiv 0$, by assumption of the Theorem)
$$\int K(x,u) f(x) \xi^*(dx) = \Lambda f(u) \tag{3}$$
- Left hand side of equivalence theorem
$$
\begin{aligned}
& c^T \int\int K(x,u) \mu^*(\mathrm{d}x) \nu^T(\mathrm{d}u) c \\
\stackrel{(2)}{=} \; & c^T M^{-1}(\xi) \int\int K(x,u) f(x) \xi(\mathrm{d}x) \nu^T(\mathrm{d}u) c \\
\stackrel{(3)}{=} \; & c^T M^{-1}(\xi) \int \Lambda f(u) \nu^T(\mathrm{d}u) c \stackrel{unbiased}{=} c^T M^{-1}(\xi) \Lambda c
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Proof (idea)

- We use
$$\mu^*(\mathrm{d}x) = M^{-1}(\xi^*)f(x)\xi^*(\mathrm{d}x), \tag{4}$$
- Right hand side of equivalence theorem (with similar arguments)
$$\begin{aligned} \Phi_c(\mu^*) &= c^T M^{-1}(\xi)\Lambda c \\ &= c^T M^{-1}(\xi)B(\xi,\xi)M^{-1}(\xi)c = D(\xi) \end{aligned}$$
- μ^* minimizes Φ_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 $\mu_\eta(\mathrm{d}x) = M^{-1}(\eta)f(x)\eta(dx)$, then

$$\begin{aligned} c^T D(\eta)c &= c^T M^{-1}(\eta)B(\eta,\eta)M^{-1}(\eta)c = \Phi_c(\mu_\eta) \\ &\geq \min_\mu \Phi_c(\mu) = \Phi_c(\mu^*) = c^T D(\xi)c. \end{aligned}$$

- Since the design ξ does not depend on the particular vector c, it follows that ξ is universally optimal.

$g_\xi \equiv 0$ is "necessary" for universal optimality

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

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

If the design ξ 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 ξ.

Remarks:

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

$$LSE + \text{optimal design} \;=\; BLUE + \text{optimal design}$$

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

Remarks:

- Integral operator on $L_2(\xi)$

$$T_K(f)(\cdot) = \int_{\mathcal{X}} K(\cdot, u) f(u) \xi(\mathrm{d}u)$$

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

$$\varphi_1, \varphi_2, \cdots$$

with positive eigenvalues

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

of the operator K

Optimal designs for kernels corresponding to integral operators

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 ξ is universally optimal!**

Example: series estimation/nonparametric regression

- Consider the regression functions

$$f_j(x) = \begin{cases} 1 & \text{if} \quad j = 1 \\ \sqrt{2}\cos(2\pi(j-1)x) & \text{if} \quad j \geq 2 \end{cases} \tag{5}$$

  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 ρ is periodic with period 1
  $\rightarrow$ **the uniform design is universally optimal!**

Example: polynomial regression

- Consider the regression functions

$$f_j(x) = x^{j-1}\ ,\ j = 1, \ldots, m+1 \tag{6}$$

on the design space $\mathcal{X} = [-1, 1]$.

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

- $\rightarrow$ **the arcsine design is universally optimal!**

$$\frac{d\xi^*}{dx} = \frac{1}{\pi\sqrt{1-x^2}}$$

Example: spherical descriptors

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

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

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

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

and P_n is the nth Legendre polynomial.

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

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

Future research: g-Optimal Designs

- **Recall:** the condition

$$g_\xi(x) = \int_{\mathcal{X}} K(x,u) f(u) \xi(du) - B(\xi,\xi) M^{-1}(\xi) f(x) \equiv 0$$

is "necessary and sufficient" for universal optimality

- A g-**optimal design** minimizes

$$||g_\xi||_2^2 = \int_{\mathcal{X}} |g_\xi(x)|^2 d\xi(x)$$

- **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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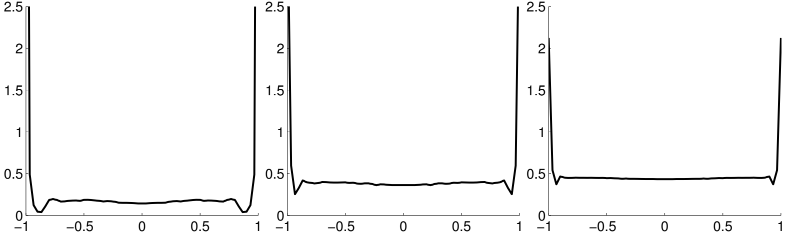
g-optimal designs for quadratic regression

- 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.

	$\lambda = 1$		$\lambda = 4$		$\lambda = 8$	
ξ	$\text{Eff}_D(\xi)$	$\text{Eff}_A(\xi)$	$\text{Eff}_D(\xi)$	$\text{Eff}_A(\xi)$	$\text{Eff}_D(\xi)$	$\text{Eff}_A(\xi)$
ξ_g^*	0.996	0.993	0.998	0.996	0.999	0.998
ξ_u	0.821	0.832	0.851	0.822	0.910	0.881

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