Optimal experimental design that minimizes the width of simultaneous confidence bands

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1. New criterion for optimal experimental design

Very brief introduction to Optimal Design

- The data $(x_i, y_i)_{1 \le i \le N} \in \mathcal{X} \times \mathbb{R}$
  ($\mathcal{X} \subset (-\infty, \infty)$ is the domain of explanatory variable x.)
- Assume a regression model

$$y_i = b^\top f(x_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2(x_i)) \text{ i.i.d.}$$

  $b \in \mathbb{R}^{n \times 1}$ (unknown), $f(x) \in \mathbb{R}^{n \times 1}$ (known), $\sigma^2(x) > 0$ (known)
- The LS: $\widehat{b} \sim N(b, \Sigma)$, where

$$\Sigma = M^{-1}, \quad M = \sum_{i=1}^{N} f(x_i) f(x_i)^\top \frac{1}{\sigma^2(x_i)} \text{ (information matrix)}$$

- "Optimal design" is to find a good $\{x_1, \ldots, x_N\} \in \mathcal{X}^N$ and hence good M, e.g., that maximizes

$$\det(\mathrm{Var}(\widehat{b}))^{-1} = \det(M) \quad \text{(D-optimal criterion)}$$

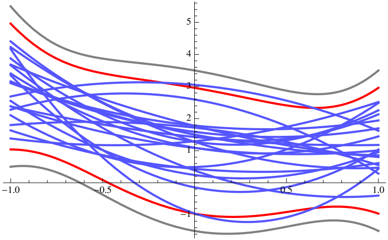
Simultaneous confidence bands

- $100(1-\alpha)\%$-simultaneous confidence band:

$$P\Big(b^\top f(x) \in \underbrace{\widehat{b}^\top f(x) \pm \|M^{-\frac{1}{2}} f(x)\| \cdot c_\alpha}_{\text{confidence band}} \ \text{for all } x \in \mathcal{X}\Big) = 1-\alpha$$

- Example of a confidence band:

$$b^\top f(x) = x^2 - x + 1, \ \ \sigma^2(x) \equiv 1, \ \ x_i = 1, 0, -1, \ \ \mathcal{X} = [-1, 1]$$



Blue	: Estimated curves (20 times)
Red	: 90% Confidence band (Naiman's volume-of-tube method)
Black	: Conservative 90% confidence band (Scheffè)

- The trajectory of the normalized regression basis vector

$$\Gamma = \left\{ \pm \frac{M^{-\frac{1}{2}} f(x)}{\|M^{-\frac{1}{2}} f(x)\|} \mid x \in \mathcal{X} \right\} \subset \mathbb{S}^{n-1} \text{ (unit sphere in } \mathbb{R}^n)$$

Let

$\mathrm{Vol}_1(\Gamma)$: 1-dim volume (length) of Γ

$\chi(\Gamma)$: the number of connected components of Γ

Proposition 1 (Naiman's (1986) volume-of-tube method)

$$P\Big(b^\top f(x) \in \widehat{b}^\top f(x) \pm \|M^{-\frac{1}{2}} f(x)\| \cdot c \ \ \textit{for all } x \in \mathcal{X} \Big)$$
$$\gtrapprox 1 - \frac{\mathrm{Vol}_1(\Gamma)}{2\pi} P(\chi_2^2 > c^2) - \frac{\chi(\Gamma)}{2} P(\chi_1^2 > c^2) \qquad (1)$$

("$\geq$" holds for all $c \geq 0$, "$\approx$" holds when c is large)

- By equating the RHS (1) to $1 - \alpha$, $c = c_\alpha$ is obtained.

Volume criterion — New optimal design criterion

- Naiman's formula (redisplay)

$$P\Big(b^\top f(x) \in \widehat{b}^\top f(x) \pm \underbrace{\|M^{-\frac{1}{2}} f(x)\| \cdot c_\alpha}_{\text{band width}} \ \text{ for all } x \in \mathcal{X}\Big)$$

$$\gtrapprox 1 - \frac{\mathrm{Vol}_1(\Gamma)}{2\pi} P\big(\chi_2^2 > c_\alpha^2\big) - \frac{\chi(\Gamma)}{2} P\big(\chi_1^2 > c_\alpha^2\big) \ (= 1 - \alpha)$$

- Propose a new criterion of optimal experimental design so that the width of confidence band is minimal.
  That is, the design minimizes $\|M^{-\frac{1}{2}} f(x)\|$ and $\mathrm{Vol}_1(\Gamma)$
- The design that minimizes $\max_{x\in\mathcal{X}} \|M^{-\frac{1}{2}} f(x)\|$ is known to be the D-optimal design (Kiefer-Wolfowitz's equivalence theorem).
- We propose the optimal design that minimizes $\mathrm{Vol}_1(\Gamma)$.

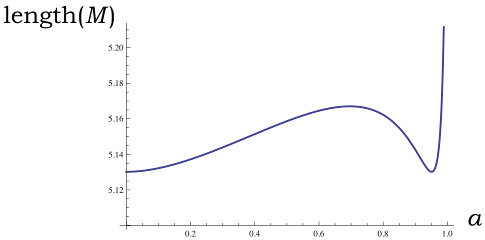
Problem is not convex!

- From now on, consider a polynomial regression (cf. Dette, et al., 1999)

$$f(x) = (1, x, \ldots, x^{n-1})^\top$$

- For example, $\mathrm{length}(M) := \mathrm{Vol}_1(M)$ for

$$M = (1-\alpha)\frac{1}{8}\begin{pmatrix}3 & 0 & 1\\ 0 & 1 & 0\\ 1 & 0 & 3\end{pmatrix} + \alpha\frac{1}{72}\begin{pmatrix}15+4\sqrt{3} & 0 & 1\\ 0 & 1 & 0\\ 1 & 0 & 7-4\sqrt{3}\end{pmatrix}$$



- The problem is not convex.

2. Polynomial regression and Möbius group action

Volume criterion — New optimal design criterion (contd)

- The length of the curve Γ is

$$\mathrm{length}(M) := \mathrm{Vol}_1(\Gamma) = \int_{\mathcal{X}} \left\| \frac{d}{dx}\left(\frac{M^{-\frac{1}{2}} f(x)}{\|M^{-\frac{1}{2}} f(x)\|} \right) \right\| dx$$

$$= \int_{\mathcal{X}} \frac{\sqrt{f^\top M^{-1} f \cdot g^\top M^{-1} g - (f M^{-1} g)^2}}{f^\top M^{-1} f} \, dx$$

where $f(x) = (1, \ldots, x^{n-1})^\top$, $g(x) = \frac{d}{dx} f(x)$

- Problem: Minimize

$$\mathrm{length}(M)$$

subject to $M \in \mathcal{M}$, where

$$\mathcal{M} = \left\{ M = \int_{\mathcal{X}} f(x) f(x)^\top dP(x) \mid P : \text{positive measure} \right\}$$

(moment cone)

- Note: Instead of $\{x_i\}_{1 \le i \le N}$, we use the design measure P.
- $\mathrm{length}(M)$ is homogeneous in M, $\mathcal{M}$ can be a cone.

Volume optimal design (polynomial regression)

- The moment cone $\mathcal{M}$ is equivalent to the set of positive definite Hankel matrices (Karlin and Studden, 1966)

$$M \in \mathcal{M} = \left\{ \begin{pmatrix} m_0 & m_1 & & m_{n-1} \\ m_1 & & \iddots & \\ & \iddots & & m_{2n-3} \\ m_{n-1} & & m_{2n-3} & m_{2n-2} \end{pmatrix}_{n\times n} \succ 0 \right\}$$

- Objective function $\mathrm{length}(M)$ is an elliptic integral

Möbius group action

- Let $\overline{\mathbb{R}} = \mathbb{R} \cup \{\pm\infty\}$. The map $\varphi : \overline{\mathbb{R}} \to \overline{\mathbb{R}}$:
$$x \mapsto \varphi(x) = \varphi(x; a, b, c, d) = \frac{ax+b}{cx+d} \quad (ad - bc \neq 0)$$
the (real) Möbius transform
- $f(x) = (1, x, \ldots, x^{n-1})^\top$
Define a matrix $A = A(a, b, c, d)$ by
$$f(\varphi(x)) = Af(x)\frac{1}{(cx+d)^{n-1}}$$
e.g., when $n = 3$,
$$\underbrace{\begin{pmatrix} 1 \\ \frac{ax+b}{cx+d} \\ (\frac{ax+b}{cx+d})^2 \end{pmatrix}}_{f(\varphi(x))} = \underbrace{\begin{pmatrix} d^2 & 2cd & c^2 \\ bd & bc+ad & ac \\ b^2 & 2ab & a^2 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix}}_{f(x)} \frac{1}{(cx+d)^2}$$
- $\mathcal{A} = \{A \mid ad - bc \neq 0\}$ forms a group (a representation of $GL(2)$)

Möbius group action (contd)

Lemma 1

If M is Hankel, then $AMA^\top$ $(A \in \mathcal{A})$ is Hankel. That is, the group $\mathcal{A}$ acts onto $\mathcal{M}$.

- We can define a equivalence relation:

$$M_1 \sim M_2 \quad \Leftrightarrow \quad M_2 = AM_1A^\top,\ \exists A \in \mathcal{A}$$

(M_1 and M_2 are on the same orbit)

Theorem 1

The group $\mathcal{A}$ remains the length $\mathrm{length}(M)$ invariant, i.e.,

$$\mathrm{length}(M_1) = \mathrm{length}(M_2) \quad \textit{if } M_1 \sim M_2$$

- We can reduce the dimension of the optimization problem.

3. Optimization over the cross-section space

Orbital decomposition

- From now on, we restricted our attention to the case $n = 3$.

Theorem 2

The moment cone $\mathcal{M}$ (= set of positive definite Hankel matrices) has an orbital decomposition

$$\mathcal{M} = \bigsqcup_{v \in (0, \frac{1}{3}]} \{M \mid M \sim M_v\}$$

where

$$M_v = \begin{pmatrix} 1 & 0 & v \\ 0 & v & 0 \\ v & 0 & 1 \end{pmatrix} \in \mathcal{M}$$

Orbital decomposition (contd)

Proof of Theorem 2.

We can show that for any $M \in \mathcal{M}$,

$$M \overset{(i)}{\sim} \begin{pmatrix} u_1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & w_1 \end{pmatrix} \overset{(ii)}{\sim} \begin{pmatrix} u_2 & 0 & v_2 \\ 0 & v_2 & 0 \\ v_2 & 0 & w_2 \end{pmatrix} \overset{(iii)}{\sim} \begin{pmatrix} 1 & 0 & v_3 \\ 0 & v_3 & 0 \\ v_3 & 0 & 1 \end{pmatrix} = M_{v_3}$$

(i) and (iii) are easy.

For (ii), we need to find $A = A(a, b, c, d)$ such that

$$A \begin{pmatrix} u_1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & w_1 \end{pmatrix} A^\top = \begin{pmatrix} u_2 & 0 & v_2 \\ 0 & v_2 & 0 \\ v_2 & 0 & w_2 \end{pmatrix}$$

by solving algebraic equations with checking resultants so that $ad - bc \neq 0$. (algebraic statistics here?) □

Optimization on the cross-section space

- The volume (length) of Γ at M_v is

$$\mathrm{length}(M_v) = \int_{-\infty}^{\infty} s(x;v)dx$$

where

$$s(x;v) = \frac{\sqrt{\frac{1-v^2}{v}}\sqrt{1+6vx^2+x^4}}{1+(\frac{1}{v}-3v)x^2+x^4}$$

(still elliptic integral...)

Theorem 3

Over $v \in (0, 1/3]$, the minimum of $\mathrm{length}(M_v)$ is attained if and only if $v = 1/3$, i.e.,

$$M = M_{1/3} = \begin{pmatrix} 1 & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 1 \end{pmatrix}$$

The minimum is $2\pi\sqrt{\frac{2}{3}}$.

Proof of Theorem 3.

Using $1/\sqrt{1+z} \geq 1 - z/2$, construct a lower bound:

$$s(x;v) \geq \underline{s}(x;v) = \frac{\sqrt{\frac{1-v^2}{v}}(1+6vx^2+x^4)}{(1+(\frac{1}{v}-3v)x^2+x^4)(1+x^2)}\Big(1+\frac{(1-3v)x^2}{(1+x^2)^2}\Big)$$

(equality iff $v = 1/3$)

$\underline{s}(x;v)$ is a rational function and the integral can be evaluated by residues.

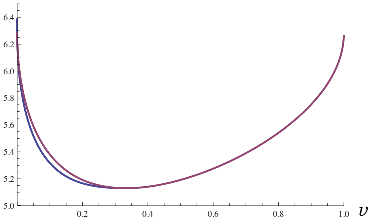
Fortunately,

$$\min_{v\in(0,1/3]} \int_{-\infty}^{\infty} \underline{s}(x;v)dx \quad \text{attains at } v = 1/3$$

and

$$\int_{-\infty}^{\infty} s(x;v)dx = \int_{-\infty}^{\infty} \underline{s}(x;v)dx \quad \text{at } v = 1/3$$

Optimization on the cross-section space (contd)



Objective function and its (integrable) lower bound

$$\text{length}(M_v) = \int_{-\infty}^{\infty} s(x;v)dx \;\geq\; \int_{-\infty}^{\infty} \underline{s}(x;v)dx$$

4. Summary and open problems

Optimal design in the polynomial regression ($n = 3$)

Theorem 4 (polynomial regression)

M is volume-mimimum optimal design iff

$$M = A M_{1/3} A^{\top}, \quad \exists A \in \mathcal{A}, \quad M_{1/3} = \begin{pmatrix} 1 & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 1 \end{pmatrix}$$

Concretely

$$M = k \begin{pmatrix} 1 & r & \frac{q^2}{3} + r^2 \\ r & \frac{q^2}{3} + r^2 & r(q^2 + r^2) \\ \frac{q^2}{3} + r^2 & r(q^2 + r^2) & (q^2 + r^2)^2 \end{pmatrix}, \quad q \neq 0, \quad k > 0$$

Proof.

$A \in \mathcal{A}$ has a decomposition

$$A(a,b,c,d) = k \underbrace{A(q,r,0,1)}_{\text{affine}} \; \underbrace{A(\pm s, \mp t, t, s)}_{O(2) \text{ (isotropy group)}}, \quad \begin{cases} s = \cos\theta \\ t = \sin\theta \end{cases}$$

Optimal design in the polynomial regression ($n = 3$) (contd)

Remark 1

It is known that

$$M_{1/3} = \begin{pmatrix} 1 & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 1 \end{pmatrix}$$

is the D-optimal information matrix.

$$\Big\{\textit{Whole designs}\Big\} \quad \textit{(4-dim)}$$
$$\supsetneq \Big\{\textit{Minimum-volume optimal designs}\Big\} \quad \textit{(2-dim)}$$
$$\supsetneq \Big\{\textit{D-optimal design}\Big\} \quad \textit{(0-dim)}$$

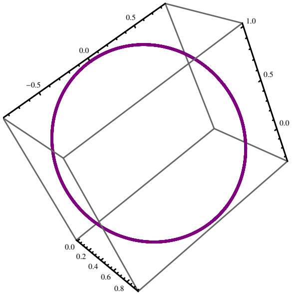
The D-optimal design is a universal optimal design that optimizes both D-criterion and volume criterion (hence, minimizes the width of simultaneous confidence bands).

Remark 2

The minimum-volume design $M \in \mathcal{M}$ is attained iff the curve

$$\Gamma_+ = \left\{ M^{-\frac{1}{2}} f(x) / \| M^{-\frac{1}{2}} f(x) \| \mid x \in \mathcal{X} \right\}$$

forms a circle.



Future topic: Multivariate extension

- $x = (x_i)^\top_{1 \le i \le p}$

$$f(x) = (1, (x_i)_{1 \le i \le p}, (x_i x_j)_{1 \le i \le j \le p}, \ldots, (x_{i_1} \cdots x_{i_d})_{1 \le i_1 \le \cdots \le i_d})^\top \in \mathbb{R}[x]^{\binom{p+d}{d}}$$

- Möbius transform $\overline{\mathbb{R}}^p \to \overline{\mathbb{R}}^p$

$$\varphi(x; A, b, c, d) = \frac{Ax + b}{c^\top x + d}, \quad A \in \mathbb{R}^{p \times p}, \quad b,\, c \in \mathbb{R}^{p \times 1}, \quad d \in \mathbb{R}$$

- "Volume preserving property" holds:

$$\mathrm{Vol}(M) = \mathrm{Vol}(AMA^\top), \quad A \in \mathcal{A},\; M \in \mathcal{M}$$

- Moment cone:

$$\mathcal{M} = \left\{ \int_{\mathcal{X} \subset \mathbb{R}^{\binom{p+d}{d}}} f(x) f(x)^\top dP(x) \mid P : \text{positive measure} \right\} = ?$$

Summary

- We proposed a new optimal design criterion — volume criterion.
- For the polynomial regression problems, the Möbius group acts on the moment cone $\mathcal{M}$, and keeps our problem invariant.
- When $n = 3$, by the optimization over cross-section space, we found the Möbius group orbit passing through the D-optimal design are minimum-volume optimal.
  (We conjecture that this is true for arbitrary n.)

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