Covariance Estimation via Fiducial Inference

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Brief history of fiducial inference

(1930)

Sir Ronald Aylmer Fisher
Proposed *fiducial inference*

(1989-2001)

- Generalized *p*-value (Tsui & Weerahndi)
- Generalized CI (Weerahndi)
- Surrogate variable method (Chiang)

Not exact!
Not unique!

Major controversy (1930-1960)

- Generalized fiducial inference
- Established asymptotic exactness
- A variety of applications to both continuous and discrete models

(2004-present)

Various applications of the generalized fiducial approach

- bioequivalence [Hannig, Abdel-Karim & Iyer (2006)]
- mixture of normal and Cauchy distributions [Glagovskiy (2006)]
- metrology [e.g. Hannig, Iyer & Wang (2007)]
- logistic regression and LD_{50} [Hannig & Iyer (2009)]
- multiple comparisons [Wandler & Hannig (2012)]
- extreme value estimation [Wandler & Hannig (2012b)]
- variance components [e.g. Cisewski & Hannig (2012)]
- wavelet regression [Hannig & Lee (2009)]
- free-knot splines [Sonderegger & Hannig (2013)]
- volatility estimation [Katsoridas & Hannig (2015+)]
- survey analysis [Liu & Hannig (2015+)]
- ...

Generalized fiducial inference (GFI) recipe

- Data generating equation (DGE)

$$\mathbf{X} = \mathbf{G}(\mathbf{U}, \xi)$$

- Given observations & independent copies of $\mathbf{U}$,

$$\mathbf{x} = \mathbf{G}(\mathbf{U}^{\star}, \xi)$$

- A functional inverse of $\mathbf{G}$

$$\lim_{\varepsilon \downarrow 0} \left[\operatorname*{argmin}_{\xi} \|\mathbf{x} - \boldsymbol{G}(\mathbf{U}^{\star}, \xi)\| \mid \{\min_{\xi} \|\mathbf{x} - \boldsymbol{G}(\mathbf{U}^{\star}, \xi)\| \leq \varepsilon\} \right] \qquad (1)$$

- Generalized fiducial distribution (GFD) := distribution of (1)

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Explicit limit

If $\mathbf{X} \in \mathbb{R}^n$ is continuous and $\xi \in \mathbb{R}^p$, the limit (1) has density [Hannig, Iyer, Lai & Lee (2015)]

$$r(\xi|\mathbf{x}) = \frac{f_{\mathbf{X}}(\mathbf{x}|\xi) J(\mathbf{x}, \xi)}{\int_{\Xi} f_{\mathbf{X}}(\mathbf{x}|\xi') J(\mathbf{x}, \xi') \, d\xi'},$$

where $J(\mathbf{x}, \xi) = D\left(\frac{d}{d\xi} \mathbf{G}(\mathbf{u}, \xi) \Big|_{\mathbf{u}=\mathbf{G}^{-1}(\mathbf{x},\xi)} \right)$

- $n = p$ gives $D(A) = |\mathrm{det} A|$
- $\|\cdot\|_2$ gives $D(A) = |\mathrm{det}(A^\top A)|^{1/2}$
  Compare to Fraser, Reid, Marras & Yi (2010)
- $\|\cdot\|_\infty$ gives $D(A) = \binom{n}{p}^{-1} \sum_{\mathbf{i}=(i_1,\ldots,i_p)} |\mathrm{det}(A)_{\mathbf{i}}|$ where $(A)_{\mathbf{i}}$ is the $p \times p$ matrix comprising of the $i_1, \ldots, i_p$th row of the $n \times p$ matrix A (Recommended)

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Some important properties of GFD

- Aways proper
- Invariant to re-parametrization (same as Jeffreys)
- If $n > p$, NOT invariant to smooth transformation of the data
- Penalty needed for model selection [Hannig, Iyer, Lai & Lee (2015+)].

GFD for covariate A

DGE:

$$Y_i = AZ_i,\ Z_i \overset{iid}{\sim} N(0, I),\ (\Sigma = AA^T).$$

GFD of A: $r(A|\mathbf{Y}) \propto J(\mathbf{Y}, A) f(\mathbf{Y}, A)$, where

$$J(\mathbf{Y}, A) = \binom{n}{p}^{-1} \sum_{\substack{\mathbf{i}=(i_1,\cdots,i_p) \\ 1\le i_1<\cdots<i_p\le n}} \left|\det\left(\frac{\partial W_{\mathbf{i}}}{\partial A}\right)\right|,$$
$$f(\mathbf{Y}, A) = (2\pi)^{-\frac{np}{2}} |\det(A)|^{-n} \exp\left[-\frac{1}{2}\mathrm{tr}\{nS_n(AA^T)^{-1}\}\right],$$

$$W_{\mathbf{i}} = (Y_{i_1}^T, \cdots, Y_{i_p}^T)^T,\ Sn = \frac{1}{n}\sum_{i=1}^{n} Y_i^T Y_i.$$

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Special Case I: no element of A is fixed at zero

$$\frac{\partial W_{\mathbf{i}}}{\partial A} = \begin{array}{c} \begin{array}{cccc} \quad B_{\mathbf{1}} \quad & \quad B_{\mathbf{2}} \quad & \quad \cdots \quad & \quad B_p \quad \end{array} \\ \begin{pmatrix} (A^{-1}Y_{i_1})^T & & & \\ & (A^{-1}Y_{i_1})^T & & \\ & & \ddots & \\ & & & (A^{-1}Y_{i_1})^T \\ \vdots & \vdots & \vdots & \vdots \\ (A^{-1}Y_{i_p})^T & & & \\ & (A^{-1}Y_{i_p})^T & & \\ & & \ddots & \\ & & & (A^{-1}Y_{i_p})^T \end{pmatrix} \end{array} \Rightarrow \begin{array}{c} \begin{array}{ccc} \quad B'_{\mathbf{1}} \quad & \quad \cdots \quad & \quad B'_p \quad \end{array} \\ \begin{pmatrix} (A^{-1}Y_{i_1})^T & & \\ \vdots & & \\ (A^{-1}Y_{i_p})^T & & \\ & \ddots & \\ & & (A^{-1}Y_{i_1})^T \\ & & \vdots \\ & & (A^{-1}Y_{i_p})^T \end{pmatrix} \end{array}$$

- Parameter space: $\mathbb{R}^{p \times p}$
- Easy calculation for $J(\mathbf{Y}, A)$
- $\Sigma \sim IW(n, nS_n)$

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Special Case II: Clique model

- Coordinates $l \& m$ of $\mathbf{Y}_i$ are correlated only if belong to the same clique
- Total k cliques with sizes $g_1, \cdots, g_k$, $\sum_{s=1}^{k} g_s = p$
- An extension of Special Case I

General Case: possible fixed zeros in A

No closed-form expression

$$r(A|\mathbf{Y}) \propto \frac{\exp\left[-\frac{1}{2}\mathrm{tr}\{nS_n(AA^T)^{-1}\}\right]}{|\det(A)|^n \binom{n}{p}} \sum_{\substack{\mathbf{i}=(i_1,\cdots,i_p)\\ 1\le i_1<\cdots<i_p\le n}} \prod_{i=1}^{p} \binom{p}{p_i} \overline{\left|\det\left(U_{\mathbf{i},i}\right)_{\mathbf{r}_i}\right|}$$

- $\overline{\left|\det\left(U_{\mathbf{i},i}\right)_{\mathbf{r}_i}\right|}$: defined by $A^{-1}Y_{i_\ell}$'s & sparse structure of A

Theorem 1 (Consistency)

If there is one-to-one correspondence between Σ and A, $r(A|\mathbf{Y})$ is asymptotically normal.

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Fiducial Bernstein von-Mises Theorem [Sonderegger & Hannig (2013)]

Conditions:

(a) the Maximum Likelihood Estimator (MLE) is asymptotically normal

(b) the Bayesian posterior distribution becomes close to that of the MLE

(c) the fiducial distribution is close to the Bayesian posterior

⋆*Conditions (a) & (b) are easy to show.*

Condition (c) holds

Proposition 1

Let $L_n(\cdot)$ be the log-likelihood with $Y_1, \cdots, Y_n$. Then for any $\delta > 0$

$$\inf_{A \notin B(A_0,\delta)} \frac{\min_{\substack{\mathbf{i}=\{i_1,\cdots,i_p\} \\ 1\le i_1<\cdots<i_p\le n}} \log f(A, \mathbf{Y}_\mathbf{i})}{|L_n(A) - L_n(A_0)|} \xrightarrow{A_0} 0, \quad as\ n \to \infty.$$

Proposition 2

Let $\mathbf{Y}_0 = (Y_1, Y_2, \cdots, Y_p)$ and $\pi(A) = E_{A_0} J(\mathbf{Y}_0, A)$. Assume that there is a one-to-one correspondence between $\Sigma = AA^T$ and A. Then the Jacobian function $J(\mathbf{Y}, A) \xrightarrow{a.s.} \pi(A)$ uniformly on compacts in A.

Clique model selection

Apply a sparse structure penalty $q(M)$ & marginalize out A,

$$r(M|\mathbf{Y}) \propto \prod_{s=1}^{k} \left[\Gamma_{g_s}\left(\frac{n}{2}\right) C_s(\mathbf{Y})(2\pi)^{\frac{g_s(g_s-1)}{2}} \left|\det S_n^s\right|^{-\frac{n}{2}} \right] \exp\left\{-q(M)\right\}$$

for clique s,

- S_n^s: $g_s \times g_s$ sample covariance matrix
- $C_s(\mathbf{Y})$: Jacobian constant
- $\Gamma_{g_s}(\frac{n}{2})$: multivariate gamma function

Clique result

Definition 1

A clique model M is **compatible** *with the true covariance matrix Σ_0, if $\Sigma_0^M = \Sigma_0$. Denote it as $M_0 \subset M$, where M_0 is the true model.*

Theorem 2

Assume the penalty $q(M)$ satisfies

i. *for any $M_0 \not\subset M$, $det\Sigma_0 < det\Sigma^M$, and $-an + q(M) - q(M_0) \to -\infty, \forall a$ as $n \to \infty$;*

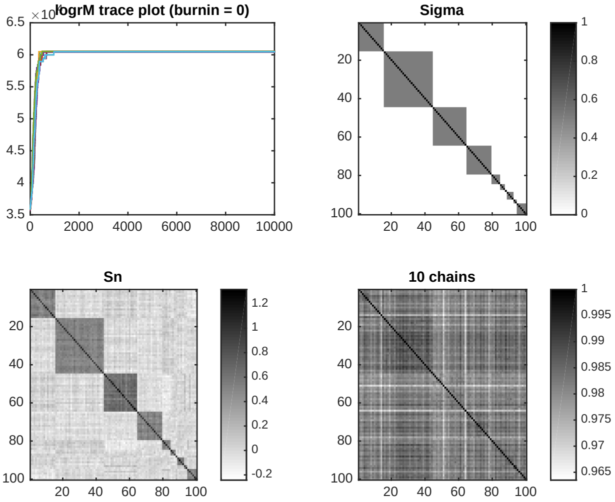
ii. *for any $M_0 \subset M$, $q(M) - q(M_0)$ is bounded.*

Then the penalized GFD

$$r(M_0|\mathbf{Y}) \xrightarrow{P} 1, \quad as\ n \to \infty$$

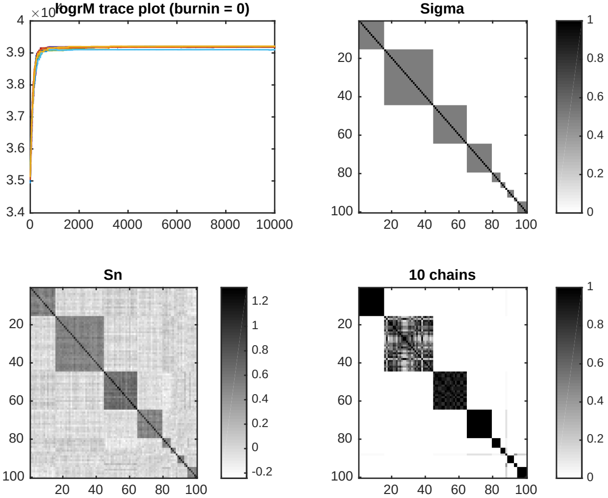
No penalty.

$q(M) = 0;\ k = 10, p = 100, n = 200.$



A minimum description length (MDL) penalty

$$q(M) = \frac{1}{3}\left(\sum_{s=1}^{k} g_s^2\right)\log n + (p+1)\log k;\ \ k = 10, p = 100, n = 200.$$



General case model selection

$$r(A|\mathbf{Y}) \propto \frac{\exp\left[-\frac{1}{2}\mathrm{tr}\{nS_n(AA^T)^{-1}\}\right]}{|\det(A)|^n \binom{n}{p}} \sum_{\substack{\mathbf{i}=(i_1,\cdots,i_p)\\ 1\le i_1<\cdots<i_p\le n}} \prod_{i=1}^{p} \binom{p}{p_i} \overline{\left|\det\left(U_{\mathbf{i},i}\right)_{\mathbf{r}_i}\right|}$$

GC 1. Known sparse structure of A.

- standard MCMC

GC 2. Sparse structure of A unknown (model selection).

- apply an MDL based penalty
- Gibbs w/ moves: update, birth, death (RJMCMC)
- adaptive birth proposal variance
  - *zeroth-order-method* [Brooks, Giudici & Roberts (2003)]

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Access general case result

Definition 2

Suppose the empirical cumulative density function is f_{ecdf}, then the **confidence curve function** f_{cc} *is defined as the following:*

$$f_{cc}(x) = \begin{cases} 2(1 - f_{ecdf}(x)), & \textit{if } f_{ecdf}(x) \geq 0.5, \\ 2f_{ecdf}(x), & \textit{otherwise.} \end{cases}$$

Various statistics: GFD, D2Sig, LogD, Eigvec angle, $\cdots$.

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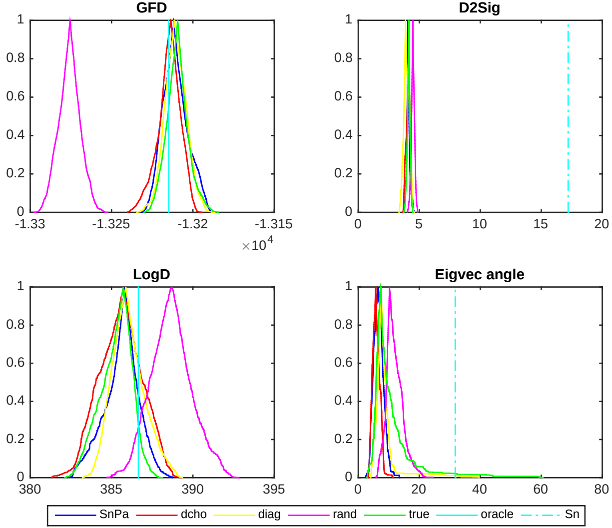
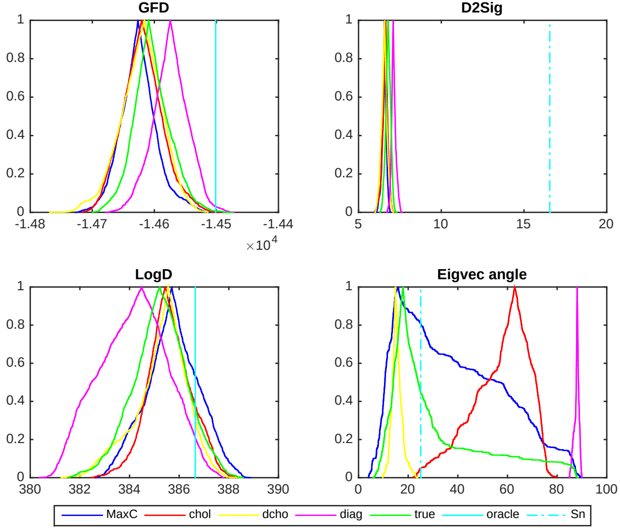
GC1: sparsity known

Confidence curves for $p = 50$, $n = 50$, $burnin = 100000$.



GC2: sparsity unknown

$p = 50$, $n = 50$, $burnin = 100000$. Same data as before.



- Recap
  - GFI does NOT require priors.
  - Functional inverse of DGE $\Rightarrow$ GFD.
  - $r(A|\mathbf{Y})$ is consistent if $A \leftrightarrow \Sigma$ is 1-to-1.
  - The clique result can be extended to $p \to \infty$, with $p/\sqrt{n} \to 0$.
  - Sample from GFD via MCMC/RJMCMC.
  - Fiducial samples $\Rightarrow$ confidence regions.
- Ongoing work
  - Improve sampling efficiency, e.g. BDMCMC instead of RJMCMC [Stephens (2000)].
  - Penalty tuning.

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Thank You!