Coverage of credible intervals under multivariate monotonicity

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- Reference: Coverage of credible intervals in Bayesian multivariate isotonic regression, *The Annals of Statistics*, Vol. 51, No 3, pages 1376–1400 (2023).

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Preliminaries

 $Y = f(X) + \varepsilon$, X univariate or multivariate, f increasing in (each component of) x.

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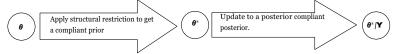
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- Consider a map that takes an element of Θ to an element of Θ_0 . This may be used to induce a prior distribution on Θ_0 , but the corresponding posterior distribution is complicated.
- The key idea is to switch the order of a map $\iota:\theta\mapsto\theta^*$ enforcing the desirable restriction, and the posterior updating, and use the induced posterior distribution to make an inference.



Traditional Bayes vs the Off-beat Bayesian Idea

Traditional Bayes



Off-beat Bayes



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- An immersion map only needs to be defined on the support of the prior/posterior. Oftentimes, priors are put using basis expansion.
 Then the immersion map will typically be a finite-dimensional optimization.

Univariate Monotone Regression

Chakraborty and G. (2021, EJS; 2021, AoS)

• A finite random series of step functions: $f(x) = \sum_{j=1}^{J} \theta_{j} \mathbb{1}((j-1)/J < x \leq j/J], \ \theta_{1}, \dots, \theta_{J}$ are the coefficients given a prior distribution, J is the number of terms.

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- Monotone projection reduces to isotonization of the θ -coefficients, for which efficient algorithms like the PAVA exist.
- Work with a deterministic choice of J, depending on the sample size
 n.

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- We shall obtain coverage of the monotone regression problem with the empirical \mathbb{L}_2 -projection-posterior, which corresponds to the weighted isotonization problem of minimizing $\sum_{j=1}^J N_j (\theta_j \theta_j^*)^2$ subject to $\theta_1^* \leq \cdots \leq \theta_J^*$, where $N_j = \sum_{i=1}^n \mathbb{1}\{(j-1)/J < X_i \leq j/J]\}$.

Limiting Coverage of a Credible interval

Let $\Delta_f^*=\arg\min\{f(t)+t^2:t\in\mathbb{R}\}$, W_1,W_2 be independent two-sided Brownian motions, $C_0=2b\left(a/b\right)^{2/3}$ with $a=\sqrt{\sigma_0^2/g(x_0)}$, $b=f_0'(x_0)/2$, g the density of X. Let \hat{f}_n be the sieve-MLE. Let $F_{a,b}^*(z|w)=\mathrm{P}(C_0\Delta_{w+W_2}^*\leq z)$.

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Theorem

- (a) for every $z \in \mathbb{R}$, $\Pi(n^{1/3}(f^*(x_0) f_0(x_0)) \le z|\mathbb{D}_n) \leadsto F_{a,b}^*(z|W_1)$;
- (b) Limiting coverage of $I_{n,\gamma}$: with $Z_B = P(\Delta_{W_1+W_2}^* \ge 0 | W_1)$, $P_0(f_0(x_0) \in I_{n,\gamma}) \to P(\gamma/2 \le Z_B \le 1 \gamma/2)$.

Note that the nuisance parameters a, b magically vanish from the limit.



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- If the target coverage is $(1-\alpha)$, starting with a $(1-\gamma)$ -credible interval, where $A(\gamma/2)=\alpha/2$, the **limiting coverage** $(1-\alpha)$ is attained exactly.



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- For instance, 93.2% equal-tailed credible interval has 95% limiting coverage.



Multivariate Monotone Regression

Wang and G. (2023, AoS).

• $Y = f(\mathbf{X}) + \varepsilon$ with $\mathbf{X} \sim G$ on $[0,1]^d$, f multivariate monotone, that is, $f(\mathbf{x}_1) \leq f(\mathbf{x}_2)$ if $\mathbf{x}_1 \leq \mathbf{x}_2$, where $\mathbf{x}_1 \leq \mathbf{x}_2$ means that $x_{1,k} \leq x_{2,k}$, $k = 1, \ldots, d$.

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- Prior: On piecewise constant functions $f = \sum_{j} \theta_{j} \mathbb{1}_{l_{j}}$ on the blocks $l_{j} = \prod_{k=1}^{d} ((j_{k} 1)/J, j_{k}/J]$ with a prior on the random heights θ_{j} .

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- Monotonicity will be ensured if the array of coefficients $\boldsymbol{\theta}$ belongs to the cone $\mathcal{C} := \{ \boldsymbol{\theta} \in \mathbb{R}^{J^d} : \theta_{j_1} \leq \theta_{j_2} \text{ if } j_1 \leq j_2 \}.$

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- Optimal \mathbb{L}_1 -contraction rate $n^{-1/(d+2)}$ using the \mathbb{L}_1 or \mathbb{L}_2 -projection posterior based on the conjugate normal prior.
- This also leads to a consistent Bayesian test as before.



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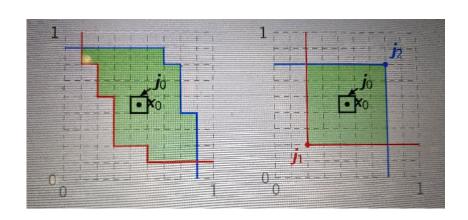
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- The clue comes from the operation used in the construction of the maxi-min estimator of Han and Zhang (2020, Ann Stat).
- A major difference with theirs is that the operation is in a discrete domain, and hence is also simpler, because of the binning through the hypercubes used in constructing the basis of step functions.



$$\bar{\iota}(f)(\mathbf{x}_0) = \min_{\mathbf{j}_0(\mathbf{x}_0) \leq \mathbf{j}_2} \max_{\substack{\mathbf{j}_1 \leq \mathbf{j}_0(\mathbf{x}_0) \\ N_{[j_1:j_2]} > 0}} \frac{\sum_{\mathbf{j} \in [\mathbf{j}_1:\mathbf{j}_2]} N_{\mathbf{j}}\theta_{\mathbf{j}}}{N_{[\mathbf{j}_1:\mathbf{j}_2]}}.$$

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• Both operations $\underline{\iota}$ and $\overline{\iota}$ are asymmetric in terms of the direction. A symmetric operation is obtained by averaging:

$$\iota(f)(\mathbf{x}_0) = (\underline{\iota}(f)(\mathbf{x}_0) + \overline{\iota}(f)(\mathbf{x}_0))/2.$$

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- Denote the images under the corresponding immersion maps by $f_*(\mathbf{x}_0)$, $f^*(\mathbf{x}_0)$, and $\tilde{f}(\mathbf{x}_0)$ respectively.
- In the univariate case, all three operations coincide and reduce to the empirical \mathbb{L}_2 -projection on monotone functions for stepwise functions given by the standard isotonization procedure for the step-heights.

• Local smoothness: let β_k be the order of the first non-zero derivative of f at \mathbf{x}_0 along the kth coordinate, that is, $\beta_k = \min_{l \geq 1} \{l : \partial_k^l f(\mathbf{x}_0) \neq 0\}.$

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- For a positive sequence $\omega_n \downarrow 0$, set $\mathbf{r}_n = (\omega_n^{1/\beta_1}, \dots, \omega_n^{1/\beta_s}, 1, \dots, 1)^T$. For any t > 0,

$$\sup_{|x_k-x_{0,k}|\leq tr_{n,k}} \left| f_0(\mathbf{x}) - f_0(\mathbf{x}_0) - \sum_{\mathbf{I}\in L} \frac{\partial^{\mathbf{I}} f_0(\mathbf{x}_0)}{\mathbf{I}!} (\mathbf{x} - \mathbf{x}_0)^{\mathbf{I}} \right| = o(\omega_n),$$

where

$$L = \{I : 0 < \sum_{k=1}^{s} I_k/\beta_k \le 1 \text{ and } I_k = 0, \text{ for } k = s+1,\dots,d\}.$$



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$$\sup_{|x_k-x_{0,k}| \leq tr_{n,k}} |f_0(x) - f_0(x_0) - \sum_{I \in L} \frac{\partial^I f_0(x_0)}{I!} (x - x_0)^I | = o(\omega_n),$$

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$$L = \{I : 0 < \sum_{k=1}^{s} I_k / \beta_k \le 1 \text{ and } I_k = 0, \text{ for } k = s+1, \dots, d\}.$$

• β_k is odd, $k \leq s$; $\partial^I f_0(\mathbf{x}_0) = 0$ if $\sum I_k/\beta_k < 1$.



Notations

Let H_1 , H_2 be independent centered Gaussian processes on $\mathbb{R}^d_{\geq 0} \times \mathbb{R}^d_{\geq 0}$ with covariance kernel

$$K(\boldsymbol{u},\boldsymbol{v})=\prod_{k=1}^s(u_k\wedge u_k'+v_k\wedge v_k')D_s(\boldsymbol{u}\wedge \boldsymbol{u}',\boldsymbol{v}\wedge \boldsymbol{v}')$$
, where

$$D_s(\boldsymbol{u} \wedge \boldsymbol{u}', \boldsymbol{v} \wedge \boldsymbol{v}') = \int_{\substack{x_k \in [(\boldsymbol{x}_0 - \boldsymbol{u})_k, (\boldsymbol{x}_0 + \boldsymbol{v})_k] \cap [0,1] \\ s+1 \leq k \leq d}} g(x_{0,1}, \dots, x_{0,s}, x_{s+1}, \dots, x_d) dx_s$$

with $D_d(\mathbf{u}, \mathbf{v}) = g(\mathbf{x}_0)$, where g is the probability density function of \mathbf{X} .

Let

$$U(\mathbf{u}, \mathbf{v}) = \frac{\sigma_0 H_1(\mathbf{u}, \mathbf{v})}{\prod_{k=1}^s (u_k + v_k) D_s(\mathbf{u}, \mathbf{v})} + \frac{\sigma_0 H_2(\mathbf{u}, \mathbf{v})}{\prod_{k=1}^s (u_k + v_k) D_s(\mathbf{u}, \mathbf{v})} + \sum_{\mathbf{l} \in L^*} \frac{\partial^{\mathbf{l}} f_0(x_0)}{(\mathbf{l} + \mathbf{1})!} \prod_{k=1}^s \frac{v_k^{l_k+1} - (-u_k)^{l_k+1}}{u_k + v_k}.$$

$$Z_* = \sup_{\substack{\boldsymbol{u} \succeq \mathbf{0} \\ u_k \leq x_{0,k} \\ s+1 \leq k \leq d}} \inf_{\substack{\boldsymbol{v} \succeq \mathbf{0} \\ v_k \leq 1 - x_{0,k} \\ s+1 \leq k \leq d}} U(\boldsymbol{u}, \boldsymbol{v}), \ Z^* = \inf_{\substack{\boldsymbol{v} \succeq \mathbf{0} \\ v_k \leq 1 - x_{0,k} \\ s+1 \leq k \leq d}} \sup_{\substack{\boldsymbol{u} \succeq \mathbf{0} \\ u_k \leq x_{0,k} \\ s+1 \leq k \leq d}} U(\boldsymbol{u}, \boldsymbol{v}).$$

Weak limit

Theorem

Let
$$\omega_n = n^{-1/(2+\sum_{k=1}^s \beta_k^{-1})}$$
. Let $J_k \gg r_{n,k}^{-1}$, for each $k=1,\ldots,d$, and $\prod_{k=1}^d J_k \ll n\omega_n$. For any $z \in \mathbb{R}$, we have
$$\Pi(\omega_n^{-1}(f_*(\mathbf{x}_0) - f_0(\mathbf{x}_0)) \leq z|\mathbb{D}_n) \rightsquigarrow \mathrm{P}(Z_* \leq z|H_1);$$

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$$\Pi(\omega_n^{-1}(f^*(\mathbf{x}_0) - f_0(\mathbf{x}_0)) \leq z | \mathbb{D}_n) \rightsquigarrow P(Z^* \leq z | H_1);$$

$$\Pi(\omega_n^{-1}(\tilde{f}(\mathbf{x}_0) - f_0(\mathbf{x}_0)) \leq z | \mathbb{D}_n) \rightsquigarrow P((Z_* + Z^*)/2 \leq z | H_1).$$

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- Tightness of the functional max/min activity within a compact domain with high probability.

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• Consider the $(1-\gamma)$ -quantile of the $\underline{\iota}$ -immersion posterior $Q_{n,\gamma}^{(1)}=\inf\{z:\Pi(f_*(\mathbf{x}_0)\leq z|\mathbb{D}_n)\geq 1-\gamma\}$, and the corresponding one-sided credible interval $(-\infty,Q_{n,\gamma}^{(1)}]$.

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- Similar statements for the other two immersion maps with corresponding changes in the limiting process.

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- Compared with the Han-Zhang procedure, the corrected intervals are significantly shorter (even the uncorrected ones are shorter), and have better coverage too, in most cases.

Thank you