Bayesian Aggregation for Extraordinarily Large Dataset

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Department Seminar
Statistics@LSE
May 19, 2017

[1] A Joint Work with Zuofeng Shang. Acknowledge NSF, ONR and Simons Foundation.

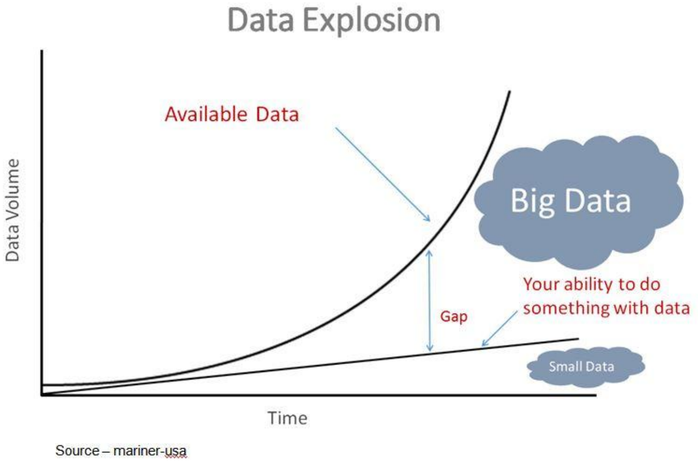
Big Data: large and complex

"There were 5 exabytes of information created between the dawn of civilization through 2003, but that much information is now created every 2 days."

— Eric Schmidt, Google CEO (2001 – 2011)

1 EB=10^{18} bytes and 1 ZB= 10^{21} bytes

Big Data: large and complex



Bayesian Aggregation

This generic aggregation procedure applies to both finite dimensional parameter and infinite dimensional parameter.

$$
\begin{array}{ccccc}
 & & \text{Subset } 1\ (n_1) & \xrightarrow{\text{Machine } 1} & R_1(\alpha) \\
\text{Big Data } (N) & \xrightarrow{\text{Divide}} & \text{Subset } 2\ (n_2) & \xrightarrow{\text{Machine } 2} & R_2(\alpha) \\
 & & \cdots & \cdots & \cdots \\
 & & \text{Subset } s\ (n_s) & \xrightarrow{\text{Machine } s} & R_s(\alpha) \\
\text{Super} \Big\Downarrow \text{machine} & & & & \text{Aggre} \Big\Downarrow \text{gate} \\
R_{\text{oracle}}(\alpha) & & & & R(\alpha)
\end{array}
$$

$R_{\text{oracle}}(\alpha)$: $(1-\alpha)$ oracle credible region constructed from the entire data (computationally prohibitive in practice, though);
$R_j(\alpha)$: $(1-\alpha)$ credible region constructed from the j-th subset.

A Series of Theoretical Questions...

- How to define an aggregation rule s.t. $R(\alpha)$ covers $(1-\alpha)$ posterior mass, with the same radius as $R_{\text{oracle}}(\alpha)$?
- How to construct a prior s.t. $R(\alpha)$ covers the true parameter (generating the data) with probability $(1-\alpha)$?
- How fast can we allow s to diverge ("splitotics theory")?
- The above tasks are particularly challenging when the parameter in consideration is infinite dimensional, which is the focus of our talk today.

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Literature Review

- In the Bayesian community, the existing statistical studies mostly focus on computational or methodological aspects of MCMC-based distributed methods;
- Nonetheless, not much effort has been devoted to *theoretically* understanding scalable Bayesian procedures especially in a general nonparametric context;
- One particular reason is the failure of Bernstein-von Mises theorem in the nonparametric setting found by Cox (1993) and Freedman (1999).

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Outline

What is Bernstein-von Mises (BvM) Theorem?

- BvM theorem[2] characterizes *asymptotic shape* of posterior distribution

$$d(\Pi(\cdot|\mathbf{D}_n), P_0(\cdot)) \longrightarrow 0 \ \text{ as } \ n \to \infty,$$

where $\Pi(\cdot|\mathbf{D}_n)$ represents a posterior measure based on sample $\mathbf{D}_n$ with size n, $P_0(\cdot)$ is a limiting probability measure, and d denotes a distance measure;

- For example, in parametric models BvM Theorem says

$$\sup_{B \in \mathcal{B}} |\Pi(B|\mathbf{D}_n) - \mathcal{N}(\widehat{\theta}_n, (nI_{\theta_0})^{-1})(B)| = o_{P^n_{\theta_0}}(1),$$

where $\mathcal{B}$ is the Borel algebra on $\mathbb{R}^d$.

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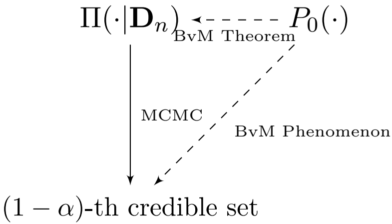
More importantly, BvM theorem implies the frequentist validity of Bayesian credible sets, called as *BvM phenomenon*, as

$$P^n_{\theta_0}(\theta_0 \in (1-\alpha)\text{-th credible set}) \to 1-\alpha.$$



Nonparametric BvM: a negative example

- Consider Gaussian sequence models:

$$Y_i = \theta_{0i} + \frac{1}{\sqrt{n}}\epsilon_i, \quad i = 1, 2, \dots,$$

where $\epsilon_i \overset{iid}{\sim} N(0,1)$. The "true" mean sequence $\{\theta_{0i}\}_{i=1}^{\infty}$ is square-summable, i.e., $\sum_{i=1}^{\infty} \theta_{0i}^2 < \infty$;

- Assign a (very innocent) Gaussian Prior:

$$\textbf{P0}: \quad \theta_i \sim N(0, i^{-2p}) \ \text{ for some } p > 1/2.$$

- Freedman (1999) demonstrated the failure of BvM:

$$P_{\theta_0}^n(\theta_0 \in (1-\alpha) \text{ credible set}) \to 0.$$

The credible set is based on ℓ^2-norm.

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A Solution: Tuning Prior

- The power of smoothing spline (Wahba, 1990)!
- We will show that nonparametric BvM theorem can be rescured under a new class of Gaussian process (GP) priors motivated by smoothing spline, named as *"tuning prior"*;
- Take Gaussian regression models as an example[3]:

$$Y_i = f_0(X_i) + \epsilon_i,\ i = 1, 2, \ldots, n,$$

where $\epsilon_i \overset{iid}{\sim} N(0,1)$ and $f \in H^m(0,1)$, a m-th order Sobolev space. Denote its log-likelihood function as

$$\ell_n(f) = -\sum_{i=1}^{n} (Y_i - f(X_i))^2/2.$$

[3] Our nonparametric BvM results hold in a general exponential family. No conjugacy is needed.

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Tuning Prior: A General Framework

- Assume that f follows a probability measure Π_λ;
- Specify Π_λ through its Radon-Nikodym derivative w.r.t. a base measure Π (also on $H^m(0,1)$) as follows:

$$\frac{d\Pi_\lambda}{d\Pi}(f) \propto \exp\left(-\frac{n\lambda}{2}J(f)\right), \qquad (1.1)$$

where $J(f)$ is a type of roughness penalty used in smoothing spline literature.

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Tuning Prior: Duality

- Based on (1.1), we have the posterior as

$$P(f|\mathbf{D}_n) := \frac{\exp(\ell_n(f))d\Pi_{\lambda}(f)}{\int_{H^m(0,1)} \exp(\ell_n(f))d\Pi_{\lambda}(f)} = \frac{\exp(\ell_{n,\lambda}(f))d\Pi(f)}{\int_{H^m(0,1)} \exp(\ell_{n,\lambda}(f))d\Pi(f)},$$

where $\ell_{n,\lambda}(f) = \ell_n(f) - n\lambda J(f)$. Smoothing spline estimate

$$\widehat{f}_{n,\lambda} := \arg \max_{f \in H^m(0,1)} \ell_{n,\lambda}(f);$$

- The name "tuning prior" now makes sense. So, we can employ GCV to select a proper tuning prior (and we did!);
- More importantly, we are able to borrow the recent advances in smoothing spline inference theory (Shang and C., 2013, *AoS*) to build a foundation of nonpara. BvM.

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Tuning Prior: Gaussian Process Construction

- To satisfy (1.1), we choose Π_λ and Π as two Gaussian measures induced by GP priors as specified below (this can be verified by applying Hájek's Lemma);
- Assign a GP prior on f, i.e., Π_λ, as follows:

$$f \sim G_\lambda(\cdot) = \sum_{\nu=1}^{\infty} w_\nu \varphi_\nu(\cdot),$$

where (recall that m is the smoothness of f_0)

$$w_\nu \sim \begin{cases} N(0,1), & \nu = 1, \ldots, m \\ N\left(0, (\rho_\nu^{1+\beta/2m} + n\lambda\rho_\nu)^{-1}\right), & \nu > m, \end{cases}$$

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- Our construction of GP prior is motivated from Wahba' Bayesian view on smoothing spline (Wahba, 1990);
- The RKHS induced by G_λ is essentially $H^{m+\beta/2}(0,1)$, where β adjusts the prior support;
- In addition, we need to assume $\beta \in (1, 2m+1)$ to guarantee $E\{J(G_\lambda, G_\lambda)\} < \infty$ such that the sample path of G_λ belongs to $H^m(0,1)$ a.s..

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Underlying Eigensystem $(\varphi_\nu(\cdot), \rho_\nu)$

- Under mild conditions, f admits a Fourier expansion:

$$f(\cdot) = \sum_{\nu=1}^{\infty} f_\nu \varphi_\nu(\cdot),$$

where $\varphi_\nu(\cdot)$'s are basis functions in $H^m(0,1)$.

- An example for (φ_ν, ρ_ν) is the following ODE solution:

$$\varphi_\nu^{(2m)}(\cdot) = \rho_\nu \varphi_\nu(\cdot),\ \ \varphi_\nu^{(j)}(0) = \varphi_\nu^{(j)}(1) = 0,\ \ j = 2, \ldots, 2m-1,$$

where φ_ν's have closed forms. This is also called as "uniform free beam problem" in physics.

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Nonparametric BvM theorem

Theorem 1

Given that $\lambda \asymp n^{-2m/(2m+\beta)}$, *we have*

$$\sup_{S \subset H^m(0,1)} |P(S|D_n) - \Pi_W(S)| = o_{P_{f_0}^n}(1),$$

where $\Pi_W(\cdot)$ *is the probability measure induced by a GP* W.

Specifications of the Limiting GP W

- Suppose that $\widehat{f}_{n,\lambda}(\cdot) = \sum_{\nu=0}^{\infty} \widehat{f}_{n,\nu}\varphi_\nu(\cdot)$;
- The mean function of W (also the approximate posterior mode of $P(\cdot|D_n)$) is

$$\widetilde{f}_{n,\lambda} := \sum_{\nu=0}^{\infty} a_{n,\nu}\widehat{f}_{n,\nu}\varphi_\nu(\cdot).$$

  Hence, $\widetilde{f}_{n,\lambda} \neq \widehat{f}_{n,\lambda}$ (but very close);
- The mean-zero GP $W_n := W - \widetilde{f}_{n,\lambda}$ is expressed as

$$W_n(\cdot) = \sum_{\nu=0}^{\infty} b_{n,\nu} z_\nu \varphi_\nu(\cdot) \ \text{ and } \ z_\nu \overset{iid}{\sim} N(0,1);$$

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Recall "Bayesian Aggregation"

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\text{Big Data } (N) & \xrightarrow{\text{Divide}} & \cdots & \cdots & \cdots \\
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R_{\text{oracle}}(\alpha) & & & & R_N(\alpha)
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$$

Note that $N = s \times n$.

Both n and s are allowed to diverge.

Uniform Nonparametric BvM Theorem

Uniform BvM theorem characterizes limit shapes of a sequence of s nonparametric posterior distributions (under proper tuning priors) as long as s does not grow too fast.

Theorem 2

Given that $\lambda \asymp N^{-2m/(2m+\beta)}$ (used in each subset with size n), we have

$$\sup_{S \subset H^m(0,1)} \max_{1 \le j \le s} |P(S|D_{j,n}) - \Pi_{W_j}(S)| = o_{P^n_{f_0}}(1)$$

as long as s does not grow faster than $N^{(\beta-1)/(2m+\beta)}$.

Aggregated Credible Interval

- The j-th credible ball is defined as

$$R_{j,n}(\alpha) = \{f \in H^m(0,1) : \|f - \widetilde{f}_{j,n}\|_2 \le r_{j,n}(\alpha)\},$$

where the radius $r_{j,n}(\alpha)$ is directly obtained via MCMC;

- The aggregated credible ball is constructed as

$$R_N(\alpha) = \{f \in H^m(0,1) : \|f - \bar{f}_{N,\lambda}\|_2 \le \bar{r}_N(\alpha)\};$$

- As will be seen, the aggregation step is through weighted averaging Fourier frequencies and weighted averaging individual radii. No additional computation is needed.

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$$R_{j,n}(\alpha) = \{f \in H^m(0,1) : \|f - \widetilde{f}_{j,n}\|_2 \leq r_{j,n}(\alpha)\},$$

  where the radius $r_{j,n}(\alpha)$ is directly obtained via MCMC;
- The aggregated credible ball is constructed as

$$R_N(\alpha) = \{f \in H^m(0,1) : \|f - \bar{f}_{N,\lambda}\|_2 \leq \bar{r}_N(\alpha)\};$$

- As will be seen, the aggregation step is through weighted averaging Fourier frequencies and weighted averaging individual radii. No additional computation is needed.

Implication of Uniform BvM Theorem

Uniform BvM shows that $R_N(\alpha)$ (asymptotically) covers $(1-\alpha)$ posterior mass and also possesses frequentist validity as long as

$$\lambda \asymp N^{-2m/(2m+\beta)} \text{ and } s = o(N^{(\beta-1/(2m+\beta))}).$$

Aggregation Details

- Aggregated center:

$$\bar{f}_{N,\lambda}(\cdot) = \sum_{\nu=1}^{\infty} a_{N,\nu} \bar{f}_\nu \varphi_\nu(\cdot) \text{ and } \bar{f}_\nu = (1/s) \sum_{j=1}^{s} \widehat{f}_{n,\nu}^{(j)};$$

- Aggregated radius:

$$\bar{r}_N(\alpha) = \sqrt{\frac{1}{N}\left[\zeta_{1,N} + \sqrt{\frac{\zeta_{2,N}}{\zeta_{2,n}}}\left(\frac{n}{s}\sum_{j=1}^{s} r_{j,n}^2(\alpha) - \zeta_{1,n}\right)\right]},$$

where

$$\zeta_{k,n} = \sum_{\nu=1}^{\infty}\left(\frac{n}{\tau_\nu^2 + n(1+\lambda\rho_\nu)}\right)^k.$$

- In fact, the aggregated radius $\bar{r}_N$ is (asymptotically) the same as that of oracle credible ball; see simulations.

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Aggregated Credible Interval

We can also aggregate individual credible intervals for linear functionals of f, denoted as $F(f)$.

- Two examples:
  - Evaluation functional: $F_z(f) = f(z)$;
  - Integral functional: $F_\omega(f) = \int_0^1 f(z)\omega(z)dz$ for a known function $\omega(\cdot)$ such as an indicator function;
- Individual credible interval for $F(f)$:

$$CI_{j,n}^F(\alpha) := \{f \in S^m(\mathbb{I}) : |F(f) - F(\widetilde{f}_{j,n})| \leq r_{F,j,n}(\alpha)\};$$

- The aggregated version is constructed as

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A Series of Theoretical Questions...

- How to define an aggregation rule s.t. $R(\alpha)$ covers $(1-\alpha)$ posterior mass, with the same radius as $R_{\text{oracle}}(\alpha)$?

  Weighted averaging individual centers (in terms of their Fourier coefficients) and radii by *analytical formula.*

- How to construct a prior s.t. $R(\alpha)$ covers the true parameter (generating the data) with probability $(1-\alpha)$?

  Pick a proper tuning prior by GCV.

- How fast can we allow s to diverge?

  s cannot grow faster than a rate jointly determined by the smoothness of f_0 and the smoothness of GP prior.

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Simulations

- Gaussian regression models:

$$Y = f_0(X) + \epsilon,$$

where $\epsilon \sim N(0,1)$ and

$$f_0(x) = 3\beta_{30,17}(x) + 2\beta_{3,11}(x),$$

where $\beta_{a,b}$ is the pdf of Beta distribution. Set $m = 2$;

- Assign a tuning prior with $\beta = 2$ and λ being selected by GCV as follows;
- Let λ_{GCV} be the GCV-selected tuning parameter with the order $N^{-2m/(2m+1)}$ by applying to the entire data (A practical formula needs to be developed here). Set λ as $\lambda_{GCV}^{(2m+1)/(2m+\beta)}$ to match with the order $\asymp N^{-2m/(2m+\beta)}$.

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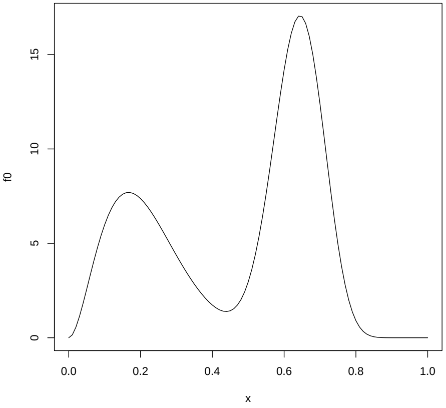

Figure 1: *Plot of the true function* f_0.

Computing Time

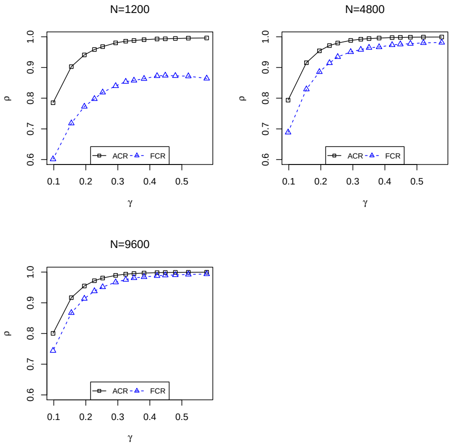

Figure 2: *ρ versus γ based on FCR and ACR, where $\rho = (T_0 - T)/T_0$, T_0 is computing time based on big data and T is the D&C time. And, $\gamma = \log s / \log N$ describes the growth of s.*

Phase Transition: Coverage Probability

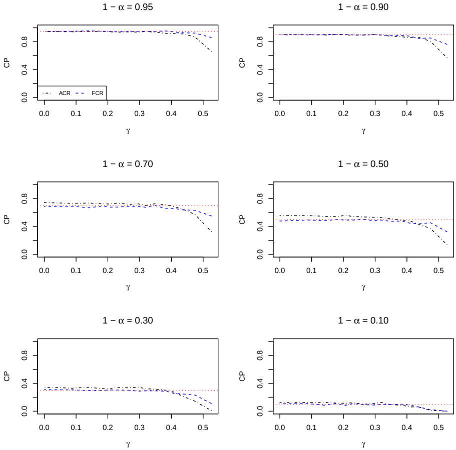

Figure 3: *Frequentist coverage probability (CP) of* $R_N(\alpha)$ *against* γ *for* $N = 2400$. *Red-dotted line indicates the position of* $1 - \alpha$.

Phase Transition: Radius

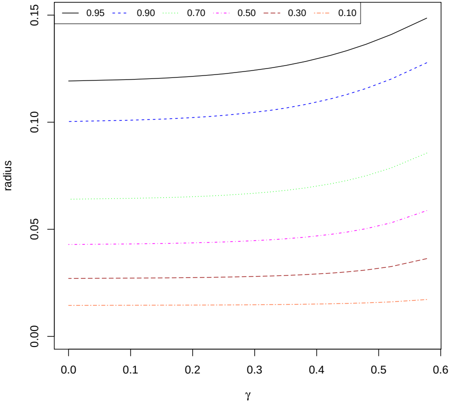

Figure 4: *Radius of $R_N(\alpha)$ against γ for various α.*

Thanks for your attention.
Questions are welcome.