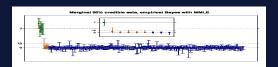
Nonparametric Bayesian Uncertainty Quantification

Lecture 2: High-dimensional Models and Sparsity

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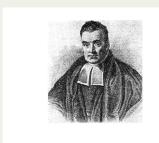
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Sparsity

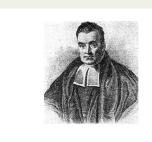
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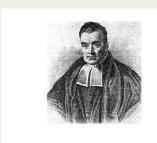


We express this in the prior, and apply the standard (full or empirical) Bayesian machine.

Parameter with prior $\theta \sim \Pi$, and data $Y^n | \theta \sim p(\cdot | \theta)$, give posterior:

$$d\Pi(\theta|Y^n) \propto p(Y^n|\theta) d\Pi(\theta).$$

A sparse model has many parameters, but most of them are (nearly) zero.



We express this in the prior, and apply the standard (full or empirical) Bayesian machine.

In this lecture sequence model: $Y^n | \theta \sim N_n(\theta, I)$.

Results extend to regression model: $Y^n \mid \theta \sim N_n(X_{n \times p}\theta, I)$ under appropriate conditions on $X_{n \times p}$.

- $\theta \in \mathbb{R}^n$ (or $\in \mathbb{R}^p$) is known to have many (almost) zero coordinates.
- n (and p) are large.

Sparsity — RNA sequencing

 $Y_{i,j}$: RNA expression count of tag $i=1,\ldots,p$ in tissue $j=1,\ldots,n$, x_j : covariate(s) of tissue j, e.g. 0 or 1 for normal or cancer.

 $Y_{i,j} \sim$ (zero-inflated) *negative binomial*, with

$$\mathrm{E}Y_{i,j} = e^{\alpha_i + \beta_i x_j}, \quad \mathrm{var} Y_{i,j} = \mathrm{E}Y_{i,j} (1 + \mathrm{E}Y_{i,j} e^{-\phi_i}).$$

Many tags i are thought to be unrelated to x_j : $\beta_i = 0$ for most i.

Constructive definition of prior Π for $\theta \in \mathbb{R}^p$:

- (1) Choose s from prior π on $\{0, 1, 2, \dots, p\}$.
- (2) Choose $S \subset \{0, 1, \dots, p\}$ of size |S| = s at random.
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We are particularly interested in π .

EXAMPLE (spike and slab)

- Choose $\theta_1, \ldots, \theta_p$ i.i.d. from $\tau \delta_0 + (1 \tau)G$.
- Put a prior on τ , e.g. Beta(1, p + 1).

This gives binomial π and product densities $g_S = \otimes_{i \in S} g$.

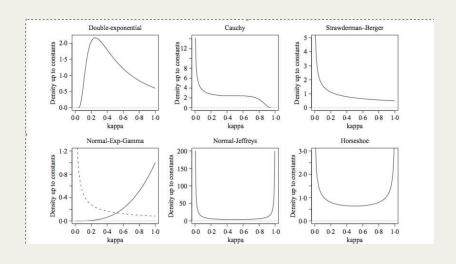
Horseshoe prior:

- (1) Generate $\tau \sim \text{Cauchy}^+(0, \sigma)$ (?)
- (2) Generate $\sqrt{\psi_1}, \ldots, \sqrt{\psi_p}$ iid from $\operatorname{Cauchy}^+(0, \tau)$.
- (3) Generate independent $\theta_i \sim N(0, \psi_i)$.

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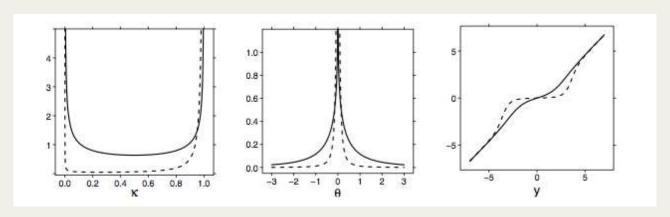
MOTIVATION: if $\theta \sim N(0,\psi)$ and $Y|\theta \sim N(\theta,1)$, then $\theta|Y,\psi \sim N\big((1-\kappa)Y,1-\kappa\big)$ for $\kappa=1/(1+\psi)$. This suggests a prior for κ that concentrates near 0 or 1.



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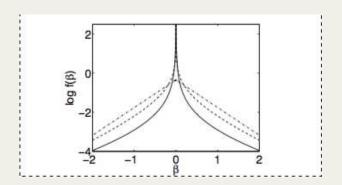


prior shrinkage factor

prior of θ_i

posterior mean of θ_i as function of Y_i

Other sparsity priors



- Bayesian LASSO: $\theta_1, \ldots, \theta_p$ iid from a mixture of Laplace (λ) distributions over $\lambda \sim \sqrt{\Gamma(a,b)}$.
- Bayesian bridge: Same but with Laplace replaced with a density $\propto e^{-|\lambda y|^{\alpha}}$.
- Normal-Gamma: $\theta_1, \ldots, \theta_p$ iid from a Gamma scale mixture of Gaussians. Correlated multivariate normal-Gamma: $\theta = C\phi$ for a $p \times k$ -matrix C and ϕ with independent normal-Gamma $(a_i, 1/2)$ coordinates.
- Horseshoe.
- Horseshoe+.
- Normal spike.
- Scalar multiple of Dirichlet.
- Nonparametric Dirichlet.
- ...

LASSO is not Bayesian

$$\hat{\theta}_{\mathsf{LASSO}} = \underset{\theta}{\operatorname{argmin}} \Big[\|Y^n - X\theta\|^2 + \lambda_n \sum_{i=1}^p |\theta_i| \Big].$$

The LASSO is the *posterior mode* for prior $\theta_i \stackrel{\text{iid}}{\sim} \text{Laplace}(\lambda_n)$, but the full posterior distribution is useless.

Trouble:

 λ must be large to shrink θ_i to 0, but small to model nonzero θ_i .

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THEOREM If $\sqrt{n}/\lambda_n \to \infty$ then

$$E_0\Pi_n(\|\theta\|_2 \lesssim \sqrt{n}/\lambda_n |Y^n) \to 0.$$

LASSO CHOICE $\lambda_n = \sqrt{2 \log n}$ gives almost no "Bayesian shrinkage".

Frequentist Bayes

Frequentist Bayes

Assume data Y^n follows a given parameter θ_0 and consider the posterior $\Pi(\theta \in \cdot | Y^n)$ as a *random measure* on the parameter set.

We like $\Pi(\theta \in \cdot | Y^n)$:

- to put "most" of its mass near θ_0 for "most" Y^n .
- to have a spread that expresses "remaining uncertainty".
- to select the model defined by the nonzero parameters of θ_0 .

We evaluate this by probabilities or expectations, given θ_0 .

Benchmarks for recovery — sequence model

$$Y^n \sim N_n(\theta, I)$$
, for $\theta = (\theta_1, \dots, \theta_n) \in \mathbb{R}^n$.

$$\|\theta\|_0 = \#(1 \le i \le n : \theta_i \ne 0),$$

$$\|\theta\|_2^2 = \sum_{i=1}^n |\theta_i|^2.$$

Frequentist benchmark: minimax rate relative to $\|\cdot\|_2$ over:

• black bodies $\{\theta: \|\theta\|_0 \leq s_n\}$:

$$\sqrt{s_n \log(n/s_n)}$$
.

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• black bodies $\{\theta: \|\theta\|_0 \leq s_n\}$:

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.

• weak ℓ_r -balls $m_r[s_n] := \{\theta : \max_i i |\theta_{[i]}|^r \le n(s_n/n)^r\}$:

$$n^{1/q}(s_n/n)^{r/q}\sqrt{\log(n/s_n)}^{1-r/q}.$$

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, for $\theta = (\theta_1, \dots, \theta_n) \in \mathbb{R}^n$.

Prior Π_n on $\theta \in \mathbb{R}^n$:

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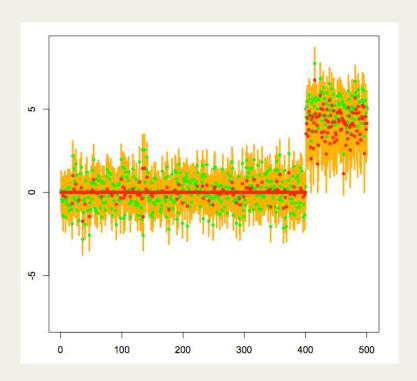
Assume

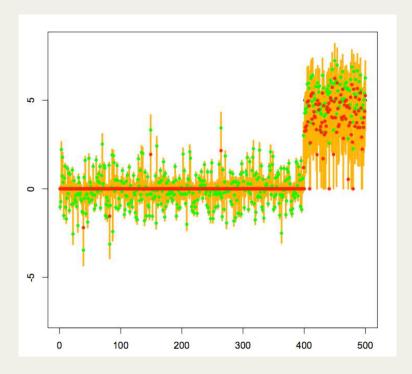
- $\pi_n(s) \le c \pi_n(s-1)$ for some c < 1, and every (large) s.
- g_S is product of densities e^h for uniformly Lipschitz $h: \mathbb{R} \to \mathbb{R}$ and with finite second moment.
- $s_n := \|\theta_0\|_0 \to 0, n \to \infty, s_n/n \to 0.$

EXAMPLES:

- complexity prior: $\pi_n(s) \propto e^{-as\log(bn/s)}$.
- spike and slab: $\theta_i \stackrel{\text{iid}}{\sim} \tau \delta_0 + (1-\tau)G$ with $\tau \sim B(1, n+1)$.

Numbers





Single data with $\theta_0=(0,\ldots,0,5,\ldots,5)$ and n=500 and $\|\theta_0\|_0=100$.

Red dots: marginal posterior medians Orange: marginal credible intervals Green dots: data points.

g standard Laplace density.

$$\pi_n(k) \propto \binom{2n-k}{n}^{0.1}$$
 (left) and $\pi_n(k) \propto \binom{2n-k}{n}$ (right).

Dimensionality of posterior distribution

THEOREM (black body)

There exists M such that

$$\sup_{\|\theta_0\|_0 \le s_n} \mathcal{E}_{\theta_0} \Pi_n \left(\theta : \|\theta\|_0 \ge M s_n | Y^n \right) \to 0.$$

Outside the space in which θ_0 lives, the posterior is concentrated in low-dimensional subspaces along the coordinate axes.

Recovery

THEOREM (black body)

For every $0 < q \le 2$ and large M,

$$\sup_{\|\theta_0\|_0 \le s_n} \mathcal{E}_{\theta_0} \Pi_n (\theta: \|\theta - \theta_0\|_q > M r_n s_n^{1/q - 1/2} |Y^n) \to 0,$$

for
$$r_n^2 = s_n \log(n/s_n) \vee \log(1/\pi_n(s_n))$$
.

If $\pi_n(s_n) \ge e^{-as_n \log(n/s_n)}$ minimax rate is attained.

Selection

$$S_{\theta} := \{1 \le i \le n : \theta_i \ne 0\}.$$

THEOREM (No supersets)

$$\sup_{\|\theta_0\|_0 \le s_n} \mathbb{E}_{\theta_0} \Pi_n(\theta; S_\theta \supset S_{\theta_0}, S_\theta \ne S_{\theta_0} | Y^n) \to 0.$$

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THEOREM (Finds big signals)

$$\inf_{\|\theta_0\|_0 \le s_n} \mathbb{E}_{\theta_0} \Pi_n \left(\theta : S_\theta \supset \{i : |\theta_{0,i}| \gtrsim \sqrt{\log n}\} | Y^n \right) \to 1.$$

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Corollary: if *all* nonzero $|\theta_{0,i}|$ are suitably big, then posterior probability of true model S_{θ_0} tends to 1.

Bernstein-von Mises theorem

THEOREM

For spike-and-Laplace(λ_n)-slab prior with $\lambda_n \sqrt{\log n}/s_n \to 0$, there are random weights \hat{w}_S ,

$$\mathbb{E}_{\theta_0} \left\| \Pi_n(\cdot | Y^n) - \sum_{S} \hat{w}_S N_{|S|}(Y_S^n, I) \otimes \delta_{S^c} \right\| \to 0.$$

THEOREM

Given consistent model selection, mixture can be replaced by $N_{|S_0|}(Y_{S_{\theta_0}},I)\otimes \delta_{S_{\theta_0}^c}$.

Corollary: Given consistent model selection, credible sets for individual parameters are asymptotic confidence sets.

Numbers: mean square errors

$\overline{p_n}$		25			50			100	
A	3	4	5	3	4	5	3	4	5
PM1	111	96	94	176	165	154	267	302	307
PM2	106	92	82	169	165	152	269	280	274
EBM	103	96	93	166	177	174	271	312	319
PMed1	129	83	73	205	149	130	255	279	283
PMed2	125	86	68	187	148	129	273	254	245
EBMed	110	81	72	162	148	142	255	294	300
HT	175	142	70	339	284	135	676	564	252
НТО	136	92	84	206	159	139	306	261	245

Average $\|\hat{\theta} - \theta\|^2$ over 100 data experiments. n = 500; $\theta_0 = (0, \dots, 0, A, \dots, A)$.

PM1, *PM2*: posterior means for priors $\pi_n(k) \propto e^{-k\log(3n/k)/10}, \binom{2n-k}{n}^{0.1}$.

PMed1, *PMed2* marginal posterior medians for the same priors *EBM*, *EBMed*: empirical Bayes mean, median for Laplace prior (Johnstone et al.) *HT*, *HTO*: thresholding at $\sqrt{2 \log n}$, $\sqrt{2 \log (n/\|\theta_0\|_0)}$.

Short Summary: Bayesian method is neither better nor worse.

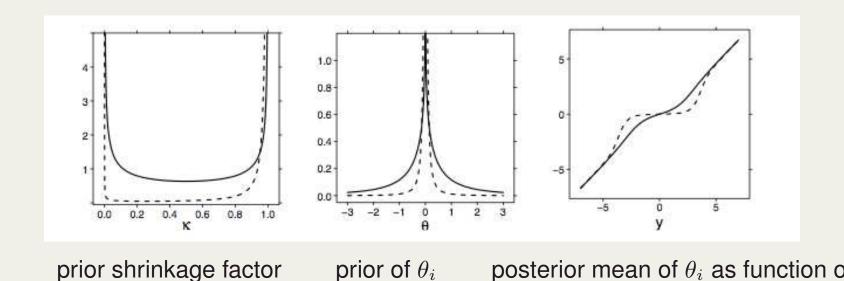
$$Y^n \sim N_n(\theta, I)$$
, for $\theta = (\theta_1, \dots, \theta_n) \in \mathbb{R}^n$.

Prior Π_n on \mathbb{R}^n :

(1) Choose "sparsity level" $\hat{\tau}$.

prior shrinkage factor

- (2) Generate $\sqrt{\psi_1}, \ldots, \sqrt{\psi_n}$ iid from $\operatorname{Cauchy}^+(0, \hat{\tau})$.
- (3) Generate independent $\theta_i \sim N(0, \psi_i)$.



posterior mean of θ_i as function of Y_i

Recovery — prechosen τ

THEOREM (black body)

If $(s_n/n)^c \le \tau_n \le C(s_n/n)\sqrt{\log(n/s_n)}$ for some c, C > 0, then for every $M_n \to \infty$,

$$\sup_{\|\theta_0\|_0 \le s_n} E_{\theta_0} \prod_n (\theta: \|\theta - \theta_0\|_2 > M_n s_n \log(n/s_n) | Y^n, \tau_n) \to 0.$$

Minimax rate $s_n \log(n/s_n)$ is attained, τ can be interpreted as sparsity level.

Credible balls — prechosen τ

For $\hat{\theta}(\tau) = E(\theta|Y^n, \tau)$ the posterior mean, set

$$\hat{C}_n(L,\tau) = \left\{\theta: \|\theta - \hat{\theta}(\tau)\|_2 \le L\hat{r}(\tau)\right\},\,$$

for $\hat{r}(\tau)$ satisfying $\Pi(\theta: \|\theta - \hat{\theta}(\tau)\|_2 \leq \hat{r}(\tau) |Y^n, \tau) = 0.95$.

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THEOREM

If $\tau_n \to 0$ such that $\tau_n \ge (s_n/n)\sqrt{\log(n/s_n)}$, then for large enough L > 0

$$\inf_{\|\theta_0\|_0 \le s_n} P_{\theta_0} (\theta_0 \in \hat{C}_n(L, \tau_n)) \ge 0.95.$$

Coverage, provided shrinkage is not too big.

For $\hat{\theta}_i(\tau) = \mathrm{E}(\theta_i | Y_i, \tau)$ the posterior mean of θ_i , set

$$\hat{C}_{ni}(L,\tau) = \left\{ \theta_i : \left| \theta_i - \hat{\theta}_i(\tau) \right| \le L \hat{r}_i(\tau) \right\},\,$$

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$$S := \{1 \le i \le n : |\theta_{0,i}| \le \tau\},\$$

$$\mathbf{M} := \{1 \le i \le n : \tau \ll |\theta_{0,i}| \le 0.999\sqrt{2\log(1/\tau)}\},\$$

L: =
$$\{1 \le i \le n: 1.001\sqrt{2\log(1/\tau)} \le |\theta_{0,i}|\}.$$

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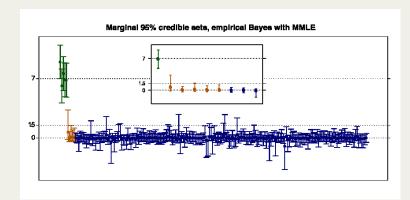
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marginal credible intervals for a single Y^n with n=200 and $s_n=10$.

 $\theta_1 = \cdots = \theta_5 = 7, \theta_6 = \cdots = \theta_{10} = 1.5$. Insert: credible sets 5 to 13.

For $\hat{\theta}_i(\tau) = E(\theta_i | Y_i, \tau)$ the posterior mean of θ_i , set

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L:=
$$\{1 \le i \le n: 1.001\sqrt{2\log(1/\tau)} \le |\theta_{0,i}|\}.$$

THEOREM For $\tau \to 0$ and any $\gamma > 0$,

$$P_{\theta_0}\left(\frac{1}{\#\mathbf{S}}\#\{i \in \mathbf{S}: \theta_{0,i} \in \hat{C}_{ni}(L_S, \tau)\} \ge 1 - \gamma\right) \to 1,$$

$$P_{\theta_0}\left(\theta_{0,i}\notin \hat{C}_{ni}(L,\tau)\right)\to 1$$
, for any $L>0$ and $i\in\mathbf{M}$,

$$P_{\theta_0}\left(\frac{1}{\#\mathbf{L}}\#\{i\in\mathbf{L}:\theta_{0,i}\in\hat{C}_{ni}(L_L,\tau)\}\geq 1-\gamma\right)\to 1.$$

Few false discoveries; most easy discoveries made.

Intermediate discoveries not made.

Estimating τ

Ad-hoc:

$$\hat{\tau}_n = \frac{\#\{|Y_i^n| \ge \sqrt{2\log n}\}}{1.1n}.$$

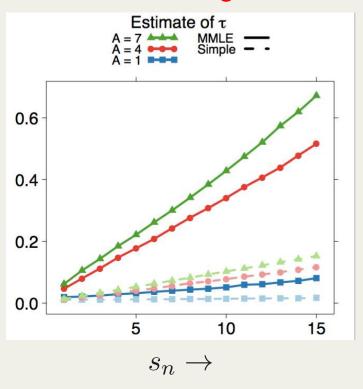
Empirical Bayes: For g_{τ} the prior of θ_i ,

$$\hat{\tau}_n = \underset{\tau \in [1/n,1]}{\operatorname{argmax}} \prod_{i=1}^n \int \phi(y_i - \theta) g_{\tau}(\theta) d\theta.$$

Full Bayes: τ set by a "hyper prior" (supported on [1/n, 1]).

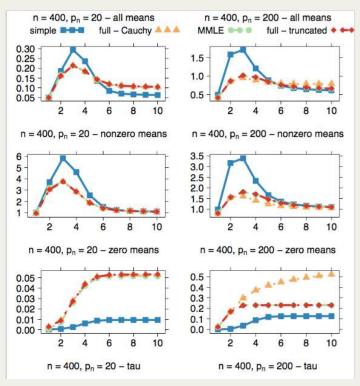
Numbers

estimating τ



 $n=100,\,s_n$ coordinates from N(0,1/4), $n-s_n$ coordinates from N(A,1).

MSE of posterior mean as function of nonzero parameter



"
$$p_n = s_n$$
"

Short summary:

Empirical Bayes and Full Bayes are similar and outperform adhoc estimator

Recovery

THEOREM (black body)

For the likelihood based empirical Bayes $\hat{\tau}_n$,

$$\sup_{\|\theta_0\|_0 \le s_n} \mathcal{E}_{\theta_0} \left[\Pi \left(\theta : \|\theta_0 - \theta\|_2 \ge M_n \sqrt{s_n \log n} | Y^n, \tau \right)_{|\tau = \widehat{\tau}_n} \right] \to 0.$$

For the full Bayes choice of τ (under mild conditions on hyper prior),

$$\sup_{\|\theta_0\|_0 \le s_n} E_{\theta_0} \Pi \Big(\theta : \|\theta_0 - \theta\|_2 \ge M_n \sqrt{s_n \log n} |Y^n\Big) \to 0.$$

Credible intervals

For $\hat{\theta}_i(\tau) = \mathrm{E}(\theta_i | Y_i, \tau)$ the posterior mean of θ_i

$$\hat{C}_{ni}(L,\tau) = \left\{ \theta_i : \left| \theta_i - \hat{\theta}_i(\tau) \right| \le L r_i(\tau) \right\},\,$$

for $r_i(\tau)$ satisfying $\Pi(\theta_i: |\theta_i - \hat{\theta}_i(\tau)| \le \hat{r}_i(\tau) |Y_i, \tau) = 0.95$.

$$\mathbf{S}_{a} := \left\{ 1 \le i \le n : |\theta_{0,i}| \le 1/n \right\},$$

$$\mathbf{M}_{a} := \left\{ 1 \le i \le n : (s_{n}/n) \sqrt{\log(n/s_{n})} \ll |\theta_{0,i}| \le 0.99 \sqrt{2 \log(n/s_{n})} \right\}.$$

$$\mathbf{L}_{a} := \left\{ 1 \le i \le n : 1.001 \sqrt{2 \log n} \le |\theta_{0,i}| \right\}.$$

THEOREM For any $\gamma > 0$ and $\|\theta_0\|_0 \le s_n$,

$$\begin{split} P_{\theta_0}\Big(\frac{1}{\#\mathbf{S}_a}\#\{i\in\mathbf{S}_a\colon\theta_{0,i}\in\hat{C}_{ni}(L_{S,\gamma},\hat{\tau}_n)\}\geq 1-\gamma\Big) &\to 1,\\ P_{\theta_0}\Big(\theta_{0,i}\notin\hat{C}_{ni}(L,\hat{\tau}_n)) &\to 1,\quad\text{for any }L>0\text{ and }i\in\mathbf{M}_a,\\ P_{\theta_0}\Big(\frac{1}{\#\mathbf{L}_a}\#\{i\in\mathbf{L}_a\colon\theta_{0,i}\in\hat{C}_{ni}(L_{L,\gamma},\hat{\tau}_n)\}\geq 1-\gamma\Big) &\to 1. \end{split}$$

If $s_n \gtrsim \log n$, the analogous is true for the hierarchical Bayes intervals.

General principle:

size of honest confidence set is determined by biggest model.

[Cai and Low, Juditzkyv& Lambert-Lacroix, 2003; Robins & van der Vaart, 2006]

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THEOREM [Li, 1987]

If $P_{\theta_0}(C_n(Y^n) \ni \theta_0) \ge 0.95$ for all $\theta_0 \in \mathbb{R}^n$, then $\operatorname{diam}(C_n(Y^n)) \gtrsim n^{-1/4}$, for some θ_0 .

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THEOREM

[Nickl, van de Geer, 2013]

If $s_{1,n} \ll s_{2,n}$ and

 $\operatorname{diam}(C_n(Y^n))$ is of order $\left((s_{i,n}/n)\log(n/s_{i,n})\right)^{1/2}$, uniformly in $\|\theta_0\|_0 \leq s_{i,n}$ for i=1,2, then

 $C_n(Y^n)$ cannot have uniform coverage over $\{\theta_0: \|\theta_0\|_0 \leq s_{2,n}\}$.

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Since the Bayesian procedure adapts to sparsity, its credible sets *cannot* be honest confidence sets.

Credible sets — impossibility of adaptation — restricting the parameter

Coverage only when θ_0 does not cause too much shrinkage.

DEFINITION [self-similarity]

For $s = \|\theta_0\|_0$ at least 0.001s coordinates of θ_0 satisfy

$$|\theta_{0,i}| \ge 1.001\sqrt{2\log(n/s)}.$$

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DEFINITION [excessive-bias restriction, Belitser & Nurushev, 2015]

$$\|\theta\|_0 \le s$$
 and $\exists \tilde{s}$ with $\tilde{s} \asymp \# \left(i: |\theta_{0,i}| \ge 1.001 \sqrt{2 \log(n/\tilde{s})}\right)$ and

$$\sum_{i:|\theta_{0,i}|\leq 1.001\sqrt{2\log(n/\tilde{s})}} \theta_{0,i}^2 \lesssim \tilde{s}\log(n/\tilde{s}).$$

Excessive-bias restriction implies self-similarity. Self-similarity allows to tighten up the sets S, M, L.

Credible balls

Empirical Bayes: Plug-in: $\hat{C}_n(L) := \hat{C}_n(L, \hat{\tau}_n)$.

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Hierarchical Bayes: For $\hat{\theta} = E(\theta | Y^n)$ the posterior mean,

$$\hat{C}_n(L) = \left\{\theta : \|\theta - \hat{\theta}\|_2 \le L\hat{r}\right\},$$

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THEOREM

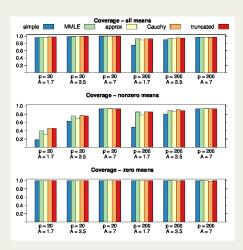
If $s_n \to 0$, for sufficiently large L,

$$\liminf_{n\to\infty} \inf_{\theta_0\in \mathsf{EBR}[s_n]} P_{\theta_0}\Big(\theta_0\in \hat{C}_n(L)\Big) \geq 1-\alpha.$$

EBR[s]: vectors θ_0 that satisfy excessive bias restriction.

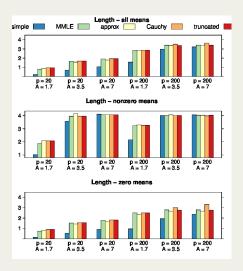
Numbers

coverage



n=400. s_n ("= p") nonzero means from $\mathcal{N}(A,1).$

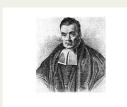
average interval length



 $n=400.\ s_n$ ("= p") nonzero means from $\mathcal{N}(A,1).$

Short summary: empirical Bayes works well

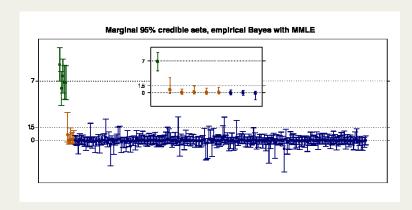
Conclusions



Bayesian sparse estimation gives excellent recovery.

For valid simultaneous credible sets need a fraction of nonzero parameters above the "universal threshold".

The danger of failing uncertainty quantification is *not* finding nonzero coordinates. Discoveries are real.



Co-authors



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Judith Rousseau



Bas Kleijn



Fengnan Gao

Compatibility and coherence

$$||X|| := \max_{j} ||X_{.,j}||.$$

Compatibility number $\phi(S)$ for $S \subset \{1, \dots, p\}$ is: $\inf_{\|\theta_{S^c}\|_1 \le 7\|\theta\|_1} \frac{\|X\theta\|_2 \sqrt{|S|}}{\|X\|\|\theta_S\|_1}$.

$$\inf_{\|\theta_{S^c}\|_1 \le 7\|\theta\|_1} \frac{\|X\theta\|_2 \sqrt{|S|}}{\|X\| \|\theta_S\|_1}.$$

Compatibility in s_n -sparse vectors means:

$$\inf_{\theta: \|\theta\|_0 \le 5s_n} \frac{\|X\theta\|_2 \sqrt{|S_{\theta}|}}{\|X\| \|\theta\|_1} \gg 0.$$

Strong compatibility in s_n -sparse vectors means: $\inf_{\theta \cdot ||\theta||_0 < 5s_n} \frac{||X\theta||_2}{||X|| ||\theta||_2} \gg 0.$

s:
$$\inf_{\theta: \|\theta\|_0 \le 5s_n} \frac{\|X\theta\|_2}{\|X\| \|\theta\|_2} \gg 0.$$

Mutual coherence means:

$$s_n \max_{i \neq j} |\operatorname{cor}(X_{.i}, X_{.j})| \ll 1.$$

Mutual coherence \Rightarrow Strong compatibility \Rightarrow Compatibility.

Mutual coherence is easy to understand and gives best recovery results, but is very restrictive.

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If $X_{i,j}$ are i.i.d. random variables, then coherence if $s_n \lesssim \sqrt{n/\log p}$.

- if $\log p = o(n)$ and $X_{i,j}$ are bounded.
- if $\log p = o(n^{\alpha/(4+\alpha)})$ and $E^{tX_{i,n}^{\alpha}} < \infty$.

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 $C = X^T X/n$: Compatibility, but no coherence if

- $C_{i,j} = \rho^{|i-j|}$, for $0 < \rho < 1$, and p = n.
- C is block diagonal with fixed block sizes.