Nonparametric Bayesian Uncertainty Quantification

Lecture 3: High-dimensional Models and Sparsity

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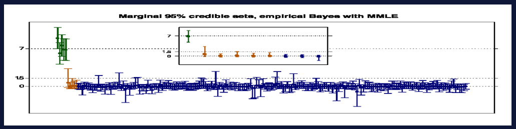
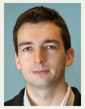


YES, Eindhoven, January 2017

Contents

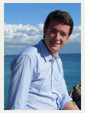
Co-authors

Sequence model & Regression



Ismael Castillo

Regression



Johannes Schmidt-Hieber

Horsehoe

Stéphanie van der Pas

Botond Szabo

Sparsity

Bayesian sparsity

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

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apply the standard (full or empirical) Bayesian machine.

Parameter with prior $\theta \sim \Pi$, and data $Y^n |\, \theta \sim p_\theta$, give posterior:

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

Bayesian sparsity

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

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

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

In both cases θ is known to have many (almost) zero coordinates, and
p and n are large.

Model selection prior

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

(1) Choose s from prior π on $\{0, 1, 2, \ldots, p\}$.
(2) Choose $S \subset \{0, 1, \ldots, p\}$ of size $|S| = s$ at random.
(3) Choose $\theta_S = (\theta_i : i \in S)$ from density g_S on $\mathbb{R}^S$ and set $\theta_{S^c} = 0$.

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We are particularly interested in π.

[Mitchell & Beachamp (88), George, George & McCulloch, Yuan, Berger, Johnstone & Silverman, Richardson et al., Johnson & Rossell, Chao Gao, ...]

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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 $g_S = \otimes_{i \in S} g$.

[Mitchell & Beachamp (88), George, George & McCulloch, Yuan, Berger, Johnstone & Silverman, Richardson et al., Johnson & Rossell, Chao Gao, ...]

Horseshoe prior

Horseshoe prior:

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

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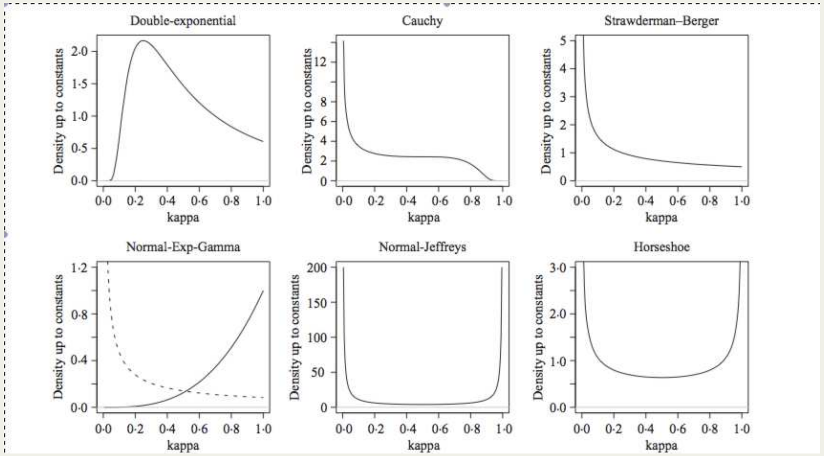
MOTIVATION: if $\theta \sim N(0, \psi)$ and $Y|\theta \sim N(\theta, 1)$,
then $\theta|Y \sim N\big((1-\kappa)Y, 1-\kappa\big)$ for $\kappa = 1/(1+\psi)$.
This suggests a prior for κ that concentrates near 0 or 1.



[Carvalho & Polson & Scott, 10.]

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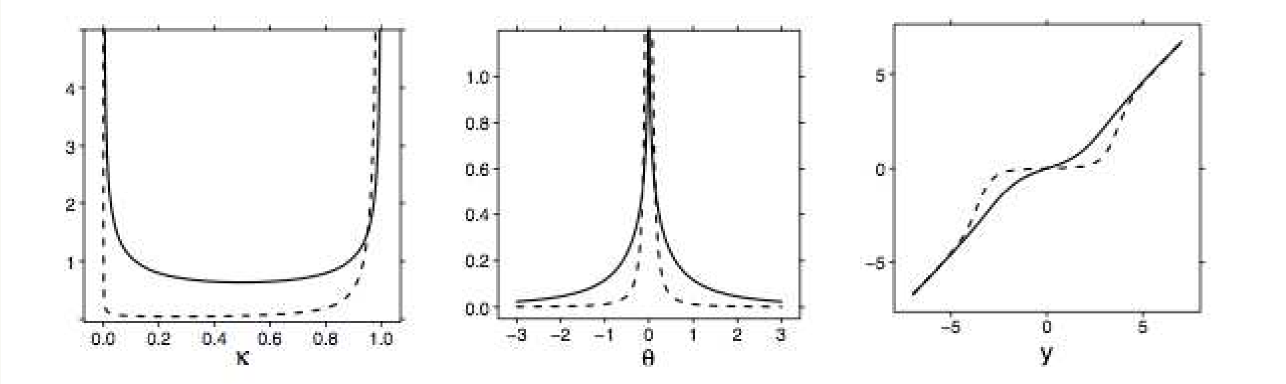
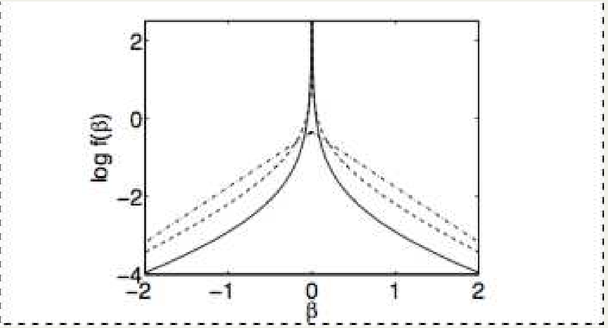


prior shrinkage factor　　prior of θ_i　　posterior mean of θ_i as function of Y_i

[Carvalho & Polson & Scott, 10.]

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*.
- ...

[Park & Casella 08, Polson & Scott, Griffin & Brown 10, 12, Carvalho & Polson & Scott, 10, George& Rockova 13, Bhattacharya et al. 12,...]

LASSO is not Bayesian

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

The LASSO is the *posterior mode* for prior $\theta_i \stackrel{\text{iid}}{\sim} \mathrm{Laplace}(\lambda_n)$,
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

$$\mathrm{E}_0 \Pi_n\big(\|\theta\|_2 \lesssim \sqrt{n}/\lambda_n \,|\, Y^n\big) \to 0.$$

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

$$\|\theta\|_0 = \#(1 \leq i \leq n \colon \theta_i \neq 0),$$
$$\|\theta\|_2^2 = \sum_{i=1}^n |\theta_i|^2.$$

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

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

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

[(if $s_n \to \infty$ with $s_n/n \to 0$.) Donoho & Johnstone, Golubev, Johnstone and Silverman, Abramovich et al.,. . .]

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

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

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

[(if $s_n \to \infty$ with $s_n/n \to 0$.) Donoho & Johnstone, Golubev, Johnstone and Silverman, Abramovich et al.,. . .]

Model Selection Prior

Model selection prior

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

(1) Choose s from prior π_n on $\{0, 1, 2, \ldots, n\}$.
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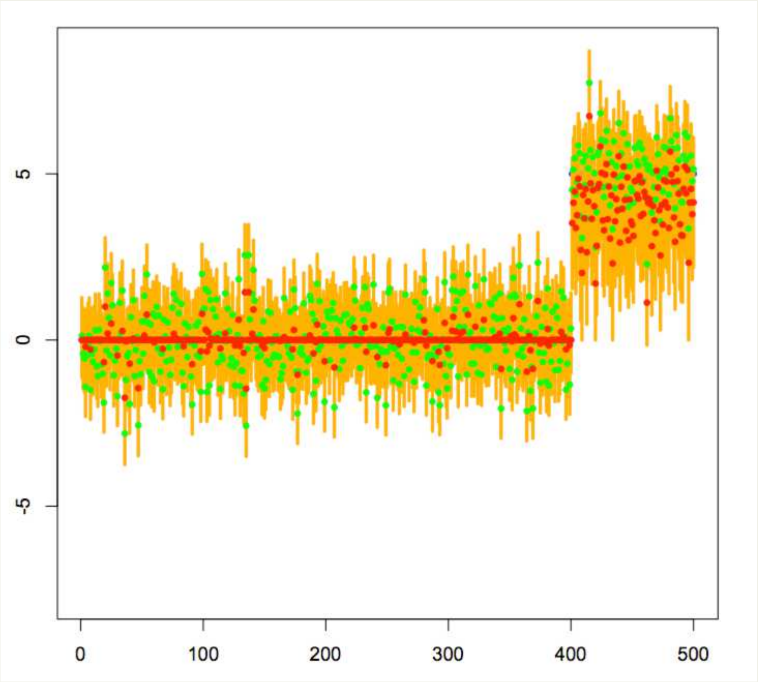
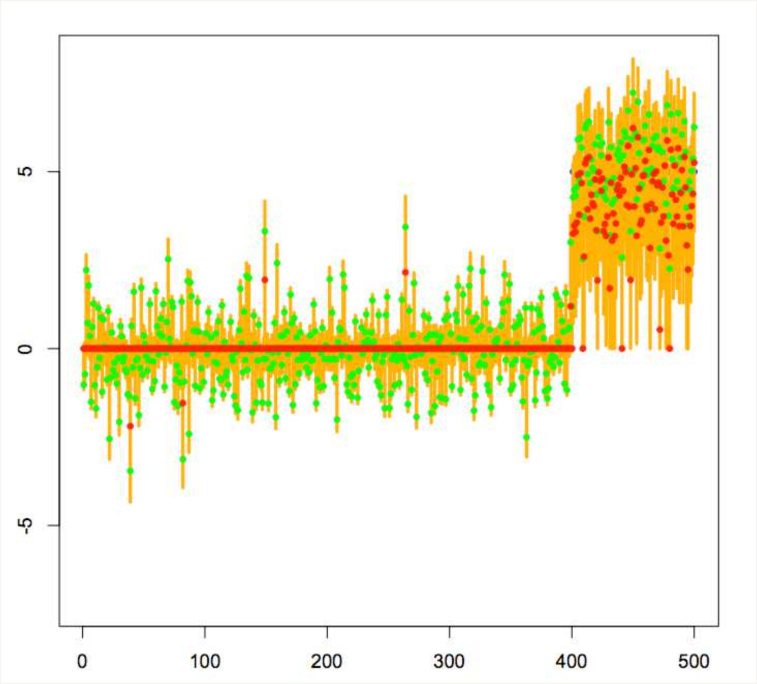
Assume

- $\pi_n(s) \leq c\,\pi_n(s-1)$ for some $c < 1$, and every (large) s.
- g_S is product of densities e^h for uniformly Lipschitz $h\colon \mathbb{R} \to \mathbb{R}$ and with finite second moment.
- $s_n, n \to \infty$, $s_n/n \to 0$. [*true number of nonzero parameters*.]

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

$\pi_n(k) \propto \binom{2n-k}{n}^{\kappa}$ for $\kappa_1 = 0.1$ (left) and $\kappa_1 = 1$ (right).

Dimensionality of posterior distribution

THEOREM *(black body)*

There exists M such that

$$\sup_{\|\theta_0\|_0 \le s_n} \mathrm{E}_{\theta_0} \Pi_n\big(\theta\colon \|\theta\|_0 \ge M s_n \,|\, Y^n\big) \to 0.$$

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 $0 < q \leq 2$ and large M,

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

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

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

Selection

$S_\theta\colon= \{1 \leq i \leq n\colon \theta_i \neq 0\}$.

THEOREM *(No supersets)*

$$\sup_{\|\theta_0\|_0 \leq s_n} \mathrm{E}_{\theta_0} \Pi_n(\theta\colon S_\theta \supset S_{\theta_0}, S_\theta \neq S_{\theta_0} \,|\, Y^n) \to 0.$$

THEOREM *(Finds big signals)*

$$\inf_{\|\theta_0\|_0 \leq s_n} \mathrm{E}_{\theta_0} \Pi_n\bigl(\theta\colon S_\theta \supset \{i\colon |\theta_{0,i}| \gtrsim \sqrt{\log n}\} \,|\, Y^n\bigr) \to 1.$$

Selection

$S_\theta := \{1 \leq i \leq n : \theta_i \neq 0\}$.

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$$\sup_{\|\theta_0\|_0 \leq s_n} \mathrm{E}_{\theta_0} \Pi_n(\theta : S_\theta \supset S_{\theta_0}, S_\theta \neq S_{\theta_0} \,|\, Y^n) \to 0.$$

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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.

Numbers: mean square errors

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
HTO	136	92	84	206	159	139	306	261	245

Average $\|\hat{\theta} - \theta\|^2$ **over** 100 **data experiments.**
$n = 500; \theta_0 = (0, \ldots, 0, A, \ldots, A)$.
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 reconstruction is neither better nor worse.

Horseshoe Prior

Horseshoe prior

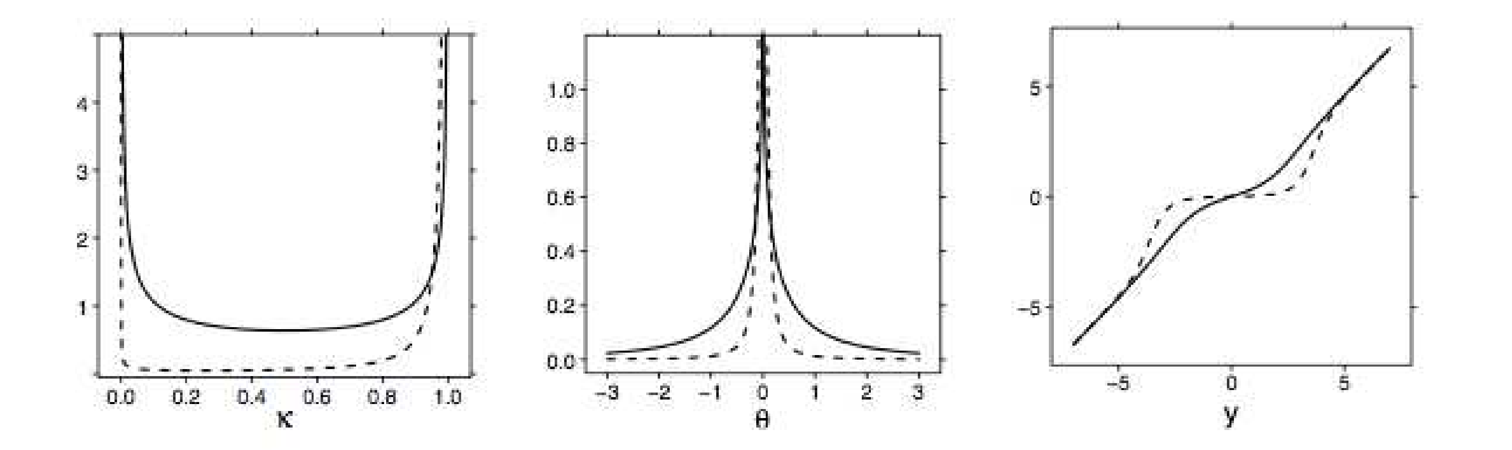
$$Y^n \sim N_n(\theta, I), \text{ for } \theta = (\theta_1, \ldots, \theta_n) \in \mathbb{R}^n.$$

Prior Π_n on $\mathbb{R}^n$:

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

(2) Generate $\sqrt{\psi_1}, \ldots, \sqrt{\psi_n}$ iid from $\mathrm{Cauchy}^+(0, \hat{\tau})$.

(3) Generate independent $\theta_i \sim N(0, \psi_i)$.



prior shrinkage factor — prior of θ_i — posterior mean of θ_i as function of Y_i

[Carvalho & Polson & Scott, 10.]

Recovery — prechosen τ

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

$$\sup_{\|\theta_0\|_0 \leq s_n} \mathrm{E}_{\theta_0} \Pi_n\big(\theta\colon \|\theta - \theta_0\|_2 > M_n s_n \log(n/s_n) \,|\, Y^n, \tau_n\big) \to 0.$$

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

Credible balls — prechosen τ

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

$$\hat C_n(L,\tau) = \Big\{\theta\colon \|\theta - \hat\theta(\tau)\|_2 \le L\hat r(\tau)\Big\},$$

with $\hat r(\tau)$ satisfying $\Pi\big(\theta\colon \|\theta - \hat\theta(\tau)\|_2 \le \hat r(\tau) \,|\, Y^n, \tau\big) = 0.95$.

THEOREM

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

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

Coverage provided shrinkage is not too big.

Credible intervals — prechosen τ

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

$$\hat C_{ni}(L,\tau) = \Big\{\theta_i\colon \big|\theta_i - \hat\theta_i(\tau)\big| \le L\hat r_i(\tau)\Big\},$$

with $\hat r_i(\tau)$ satisfying $\Pi\big(\theta_i\colon |\theta_i - \hat\theta_i(\tau)| \le \hat r_i(\tau) \,|\, Y_i, \tau\big) = 0.95$.

$$\begin{aligned}
\mathbf{S}&:= \{1 \le i \le n\colon |\theta_{0,i}| \le \tau\},\\
\mathbf{M}&:= \{1 \le i \le n\colon \tau \ll |\theta_{0,i}| \le 0.99\sqrt{2\log(1/\tau)}\},\\
\mathbf{L}&:= \{1 \le i \le n\colon 1.01\sqrt{2\log(1/\tau)} \le |\theta_{0,i}|\}.
\end{aligned}$$

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

$$P_{\theta_0}\Big(\frac{1}{\#\mathbf{S}}\#\{i \in \mathbf{S}\colon \theta_{0,i} \in \hat C_{ni}(L_S,\tau)\} \ge 1-\gamma\Big) \to 1,$$

$$P_{\theta_0}\big(\theta_{0,i} \notin \hat C_{ni}(L,\tau)\big) \to 1, \quad \text{for any } L > 0 \text{ and } i \in \mathbf{M},$$

$$P_{\theta_0}\Big(\frac{1}{\#\mathbf{L}}\#\{i \in \mathbf{L}\colon \theta_{0,i} \in \hat C_{ni}(L_L,\tau)\} \ge 1-\gamma\Big) \to 1.$$

Credible intervals — prechosen τ

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

$$\hat{C}_{ni}(L, \tau) = \Big\{\theta_i \colon \big|\theta_i - \hat{\theta}_i(\tau)\big| \leq L\hat{r}_i(\tau)\Big\},$$

with $\hat{r}_i(\tau)$ satisfying $\Pi\big(\theta_i \colon |\theta_i - \hat{\theta}_i(\tau)| \leq \hat{r}_i(\tau) | Y_i, \tau\big) = 0.95$.

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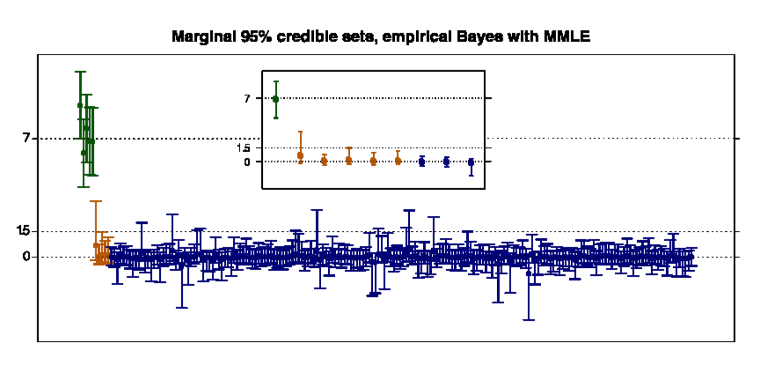


marginal credible intervals for a single Y^n with $n = 200$ and $s_n = 10$.
$\theta_1 = \cdots = \theta_5 = 7$ (green), $\theta_6 = \cdots = \theta_{10} = 1.5$ (orange). Insert: credible sets 5 to 13.

Estimating τ

Ad-hoc:

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

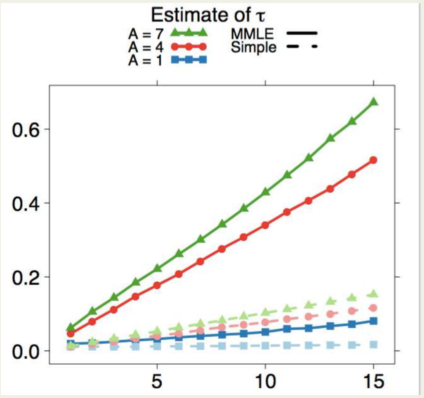
Empirical Bayes: For g_τ the prior of θ_i,

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

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

Numbers

estimating τ



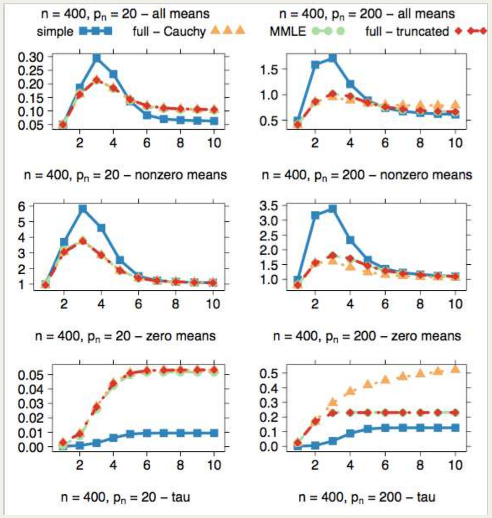
$s_n \to$

$n = 100$, 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



"$p_n = s_n$"

Empirical Bayes and Full Bayes are similar and outperform ad-hoc estimator

Recovery

THEOREM *(black body)*
For the likelihood based empirical Bayes $\hat{\tau}_n$,

$$\sup_{\|\theta_0\|_0 \le s_n} \mathrm{E}_{\theta_0}\Big[\Pi\Big(\theta\colon \|\theta_0-\theta\|_2 \ge M_n\sqrt{s_n \log n} \,|\, Y^n, \tau\Big)_{|\tau=\hat{\tau}_n}\Big] \to 0.$$

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

$$\sup_{\|\theta_0\|_0 \le s_n} \mathrm{E}_{\theta_0}\Pi\Big(\theta\colon \|\theta_0-\theta\|_2 \ge M_n\sqrt{s_n \log n} \,|\, Y^n\Big) \to 0.$$

Credible intervals

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

$$\hat{C}_{ni}(L, \tau) = \Big\{\theta_i\colon \big|\theta_i - \hat{\theta}_i(\tau)\big| \leq L\hat{r_i(\tau)}\Big\},$$

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

$$\mathbf{S}_a\colon = \big\{1 \leq i \leq n\colon |\theta_{0,i}| \leq 1/n\big\},$$
$$\mathbf{M}_a\colon = \big\{1 \leq i \leq n\colon (s_n/n)\sqrt{\log(n/s_n)} \ll |\theta_{0,i}| \leq 0.99\sqrt{2\log(n/s_n)}\big\}.$$
$$\mathbf{L}_a\colon = \big\{1 \leq i \leq n\colon 1.01\sqrt{2\log n} \leq |\theta_{0,i}|\big\}.$$

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

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

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

Credible sets — impossibility of adaptation

General principle: the size of an honest confidence set is determined by the biggest model. [Cai and Low, Juditzkyv& Lambert-Lacroix, 2003; Robins & van der Vaart, 2006]

THEOREM [Li, 1987]
If $C_n(Y)$ satisfies $P_{\theta_0}(C_n(Y) \ni \theta_0) \geq 0.95$ for all $\theta_0 \in \mathbb{R}^n$, then $\mathrm{diam}(C_n(Y)) \gtrsim n^{-1/4}$, for some θ_0.

THEOREM [Nickl, van de Geer, 2013]
If $s_{1,n} \ll s_{2,n}$ and $\mathrm{diam}(C_n(Y))$ is of order $\big((s_{i,n}/n)\log(n/s_{i,n})\big)^{1/2}$, uniformly in $\|\theta_0\|_0 \leq s_{i,n}$ for $i = 1, 2$, then $C_n(Y)$ 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 $0.02s$ coordinates of θ_0 satisfy

$$|\theta_{0,i}| \geq 1.01\sqrt{2\log(n/s)}.$$

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DEFINITION [excessive-bias restriction, Belitser & Nurushev, 2015]
$\|\theta\|_0 \leq s$ and $\exists \tilde{s}$ with $\tilde{s} \asymp \#\big(i\colon |\theta_{0,i}| \geq 1.01\sqrt{2\log(n/\tilde{s})}\big)$ and

$$\sum_{i:|\theta_{0,i}|\leq 1.01\sqrt{2\log(n/\tilde{s})}} \theta_{0,i}^2 \lesssim \tilde{s}\log(n/\tilde{s}).$$

Excessive-bias restriction implies self-similarity.
Self-similarity allows to tighten up the sets $\mathbf{S}, \mathbf{M}, \mathbf{L}$.

Credible balls

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THEOREM

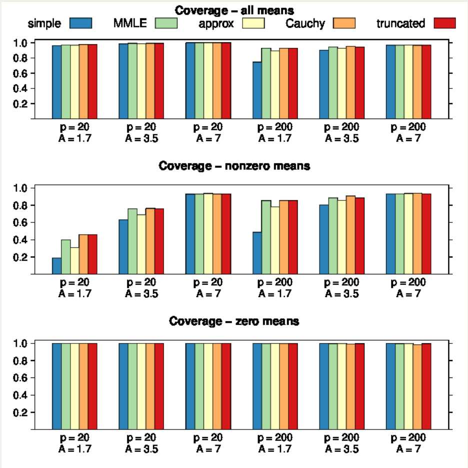
If $s_n \to 0$, for sufficiently large L,

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

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

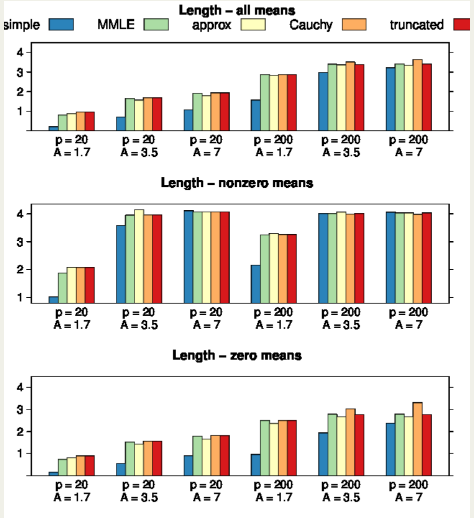
Numbers

coverage



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

average interval length



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

Conclusions

Bayesian sparse estimation gives excellent recovery.

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

The danger of failing uncertainty quantification is not finding nonzero coordinates.