Posterior contraction in nonparametric inverse problems

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Joint work with

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There is a catch...

- "Classical" theory of posterior contraction does not give interesting results ("inverseness")

Frequentist vs. Bayesian

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- Put a prior on f
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Choosing a prior can be viewed as choosing or tuning the estimation procedure

Pragmatic Bayesian

How does the posterior behave from frequentist perspective?

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Posterior contraction rate

The posterior $\Pi_n(\,\cdot\,|Y^{(n)})$ is said to contract at f_0 at rate $\varepsilon_n \downarrow 0$, if

$$\Pi_n(f : d(f, f_0) \geq M_n\varepsilon_n|Y^{(n)}) \to 0,$$

in $P_0^{(n)}$-probability, for every $M_n \to \infty$ as $n \to \infty$.

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in $P_0^{(n)}$-probability, for every $M_n \to \infty$ as $n \to \infty$.

There exist point estimators based on the posterior that also attain this rate (i.e., posterior mean or the centre of a ball capturing enough posterior mass).

General posterior contraction theorems

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General theory relies on specific, yet often natural, distances.

Wrong distance

Let $Y = (Y_1, Y_2, \dots)$

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$$Y_i = \kappa_i f_i + \frac{1}{\sqrt{n}} Z_i, \qquad i = 1, 2, \dots.$$

For any $f \in \ell_2$, and $\kappa \in \ell_2$ let $Kf = (\kappa_1 f_1, \kappa_2 f_2, \dots)$.

The natural distance between Kf_1 and Kf_2 (also from posterior contraction point of view)

$$\|Kf_1 - Kf_2\|^2 = \sum_{i=1}^{\infty} |\kappa_i f_{i,1} - \kappa_i f_{i,2}|^2$$

Wrong distance and posterior contraction

When $|\kappa_i| \downarrow 0$, even if $\|Kf - Kf_0\|$ is small, $\|f - f_0\|$ can be large.

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In general, there is no C such that

$$d(f, f_0) \leq Cd(Kf, Kf_0).$$

Therefore, we cannot say anything about

$$\Pi_n(d(f, f_0) \gtrsim \widetilde{\varepsilon}_n | Y^{(n)}) \to 0$$

based on

$$\Pi_n(d(Kf, Kf_0) \gtrsim \varepsilon_n | Y^{(n)}) \to 0.$$

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Bayes should work and does work. Putting a prior is natural way of specifying a degree of regularization.

No general theory = direct evaluation of the posterior and its properties.

Sequence setting

We observe

$$Y_i = \kappa_i f_i + \frac{1}{\sqrt{n}} Z_i, \qquad i = 1, 2, \dots,$$

and put a product prior $\Pi = \bigotimes N(0, \lambda_i)$ on the sequence $f = (f_i)$.

We say that the true f_0 is Sobolev β-smooth if $\sum i^{2\beta} f_{0,i}^2 < \infty$.

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Posterior rate of contraction

- $\lambda_i = i^{-1-2\alpha}$, $\kappa_i \asymp i^{-p}$, $\alpha > 0$, $p \geq 0$: $n^{-\frac{\alpha \wedge \beta}{1+2\alpha+2p}}$
- $\lambda_i = i^{-1-2\alpha}$, $\kappa_i \asymp \exp(-\gamma i^p)$, $\alpha, \gamma > 0$, $p \geq 1$: $(\log n)^{-\frac{\alpha \wedge \beta}{p}}$
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K, van der Vaart, van Zanten (2011, 2013), Florens and Simoni (2012, 2013), Agapiou et al. (2013, 2014), Ray (2013)

Getting the right α: Adaptation in mildly ill-posed problem

Recall

$$\Pi_\alpha = \bigotimes_i N(0, i^{-1-2\alpha})$$

where now we consider α a hyperparameter.

Getting the right α: Adaptation in mildly ill-posed problem

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In the setting described before

$$f|\alpha \sim \Pi_\alpha = \bigotimes_i N(0, i^{-1-2\alpha}) \qquad \text{and} \qquad Y|(f,\alpha) \sim \bigotimes_i N(\kappa_i f_{0,i}, n^{-1}),$$

hence

$$Y|\alpha \sim \bigotimes_i N(0, i^{-1-2\alpha}\kappa_i^{-2} + n^{-1}).$$

Empirical and hierarchical Bayes

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Empirical Bayes posterior

Replace α by the maximizer $\hat{\alpha}_n$ of the likelihood

$$\Pi_{\hat{\alpha}_n}(\,\cdot\,|Y) = \Pi_\alpha(\,\cdot\,|Y)\Big|_{\alpha=\hat{\alpha}_n}.$$

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Hierarchical Bayes

We use a prior $\lambda(\alpha)$ on α and then the full hierarchical prior is given by

$$\Pi = \int_0^\infty \lambda(\alpha)\Pi_\alpha \, d\alpha$$

Integration example

The Volterra operator

We observe the process $Y = (Y_t : t \in [0, 1])$

$$Y_t = \int_0^t \int_0^s f(u)\, du\, ds + \frac{1}{\sqrt{n}} W_t,$$

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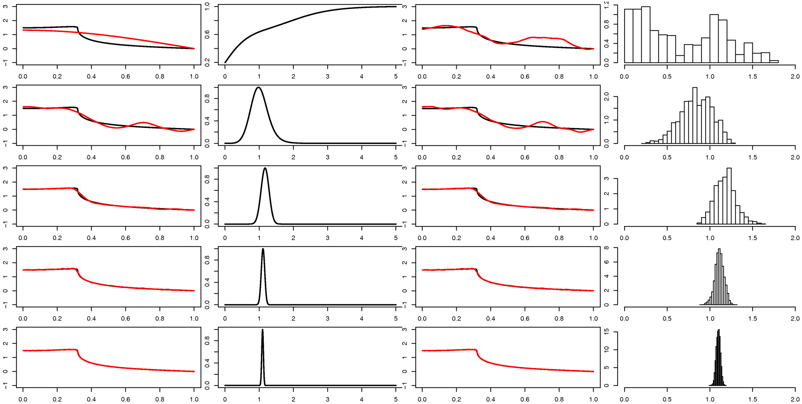
Spectral decomposition of the Volterra operator

The eigenvalues and eigenfunctions of $K^T K$ are

$$\kappa_i = \frac{1}{(i+1/2)\pi} \asymp i^{-1}, \quad e_i(x) = \sqrt{2}\cos\big((i+1/2)\pi x\big), \quad i = 0, 1, 2, \ldots.$$

Empirical and hierarchical Bayes



Black curve – true f_0, red curve – posterior mean

$n = 10^3, 10^5, 10^7, 10^9$ and 10^{11} (top to bottom)

Adaptive Bayes in mildly ill-posed problems

Let

$$\|f\|_\beta^2 = \sum_i i^{2\beta} f_i^2.$$

Theorem (K, Szabó, van der Vaart, van Zanten, 2012-2016)

For every $R > 0$ *and* $M_n \to \infty$

$$\sup_{\|f_0\|_\beta \le R} \mathrm{E}_0 \Pi_{\hat{\alpha}_n}\Big(\|f - f_0\| \ge M_n L_n\, n^{-\frac{\beta}{1+2\beta+2p}} \,|Y\Big) \to 0,$$

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where $L_n = (\log n)^2 (\log\log n)^{1/2}$ *is a slowly varying term.*

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up to a slowly varying term

Towards more general results

Let Kf denote the transformed parameter of interest f, and data by $Y \sim P_{Kf}$

Here $K : \mathscr{F} \ni f \mapsto Kf \in K\mathscr{F}$, d and d_K denote some metrics on $\mathscr{F}$ and $K\mathscr{F}$

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Problems with general theory

- rates for $d_K\big(Kf_1, Kf_2\big)$ rather than $d\big(f_1, f_2\big)$
- when the problem is ill-posed, then $d_K\big(Kf_1, Kf_2\big)$ and $d\big(f_1, f_2\big)$ are not equivalent

$$\sup\Big\{d\big(f_1, f_2\big) \,:\, f_1, f_2 \in \mathscr{F} \;\text{ s.t. }\; d_K\big(Kf_1, Kf_2\big) \leq \delta\Big\} = \infty$$

Towards more general results

Simple idea

Consider sequence of sets S_n such that

$$\sup\Big\{d\big(f,f_0\big) : f \in S_n \ \text{ s.t. } \ d_K\big(Kf,Kf_0\big) \leq \delta\Big\} < \infty$$

Simple observation

Note that the prior in the previous examples did not depend on the inverse problem K, i.e., the sequence κ_i.

Standard choice of S_n

In the sequence setting S_n could be

$$S_n = \left\{ f \in \ell_2 : \sum_{i > k_n} f_i^2 \leq c\rho_n^2 \right\},$$

for given sequences of positive numbers $k_n \to \infty$ and $\rho_n \to 0$ and a constant $c > 0$.

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If f_0 is such that for some sequence (s_i)

$$\sum_{i=1}^{\infty} f_{0,i}^2 s_i^{-2} < \infty,$$

then

$$\sup \Big\{ d(f, f_0) : f \in S_n \text{ s.t. } d_K(Kf, Kf_0) \le \delta \Big\} \lesssim \kappa_{k_n}^{-1}\delta + \rho_n + s_{k_n}.$$

Modulus of continuity and the contraction theorem

Let

$$\omega(S_n, f_0, d, d_K, \delta) = \sup\Big\{ d(f, f_0) : f \in S_n \;\text{ s.t. }\; d_K(Kf, Kf_0) \leq \delta \Big\}$$

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Theorem (K and Salomond, 201?)

Let $\varepsilon_n \to 0$ and let Π be a prior distribution for f such that

$$\mathrm{E}_0 \Pi(S_n^c \mid Y) \to 0$$

for some sequence of sets (S_n), $S_n \subset \mathscr{F}$, and

$$\mathrm{E}_0 \Pi\Big(d\big(Kf, Kf_0\big) \ge M_n \varepsilon_n \,\big|\, Y\Big) \to 0,$$

for any $M_n \to \infty$. Then

$$\mathrm{E}_0 \Pi\Big(d\big(f, f_0\big) \ge \omega(S_n, f_0, d, d_K, M_n \varepsilon_n) \,\big|\, Y\Big) \to 0.$$

Remaining posterior mass condition

Remaining posterior mass condition: $\mathrm{E}_0 \Pi\big(S_n^c \mid Y\big) \to 0$

Lemma (Lemma 1 in Ghosal and van der Vaart, 2007)

Let $\varepsilon_n \to 0$ and let (S_n) be a sequence of sets $S_n \subset \mathcal{F}$. If Π is the prior distribution on f satisfying

$$\frac{\Pi(S_n^c)}{\Pi(B_n(Kf_0, \varepsilon_n))} \lesssim \exp(-2n\varepsilon_n^2),$$

then

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Note that in the denominator we have the usual prior mass condition for the posterior contraction in the direct problem of recovering Kf.

Example 0: mildly ill-posed sequence setting

If f is Sobolev β-smooth, then Kf is Sobolev $(\beta + p)$-smooth.

The prior Π_α induces the prior $\bigotimes N(0, i^{-1-2\alpha-2p})$ on Kf.

Already Zhao (2000), and Belitser and Ghosal (2003) showed that in this case the posterior contracts at rate

$$n^{-\frac{(\alpha\wedge\beta)+p}{1+2\alpha+2p}}.$$

Example 0: mildly ill-posed sequence setting

Known:

$$\mathrm{E}_0\Pi\Big(\|Kf - Kf_0\| \geq M_n n^{-\frac{(\alpha\wedge\beta)+p}{1+2\alpha+2p}} \mid Y\Big) \to 0.$$

By taking $S_n = \Big\{f \in \ell_2 : \sum_{i>k_n} f_i^2 \leq c\rho_n^2\Big\}$ with

$$k_n = n^{\frac{1}{1+2\alpha+2p}}, \quad \rho_n = n^{-\frac{(\alpha\wedge\beta)}{1+2\alpha+2p}},$$

we get

$$\begin{aligned}\omega(S_n, f_0, \|\cdot\|, \|\cdot\|, M_n\varepsilon_n) &\lesssim \kappa_{k_n}^{-1}\delta + \rho_n + s_{k_n} \\ &\lesssim M_n n^{\frac{p}{1+2\alpha+2p}} \cdot n^{-\frac{(\alpha\wedge\beta)+p}{1+2\alpha+2p}} + n^{-\frac{(\alpha\wedge\beta)}{1+2\alpha+2p}} + n^{-\frac{\beta}{1+2\alpha+2p}} \lesssim M_n n^{-\frac{(\alpha\wedge\beta)}{1+2\alpha+2p}}.\end{aligned}$$

Example 1: Numerical differentiation

For all $f \in L_1([0, 1])$ define the operator K

$$Kf(x) = \int_0^x f(t)\,dt, \qquad \text{for } x \in [0, 1]$$

Note that the operator K is no longer defined on the Hilbert space. (No SVD)

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Consider the inverse regression problem

$$Y_i = Kf(x_i) + \sigma\epsilon_i, \qquad \epsilon_i \overset{iid}{\sim} N(0,1), \qquad i = 1,\ldots,n,$$

where the design points $x_1, x_2, \ldots, x_n \in [0,1]$ are fixed.

Example 1: Numerical differentiation

Prior

We put a prior on f such that the induced prior on Kf is well known, and we use B-spline basis $(B_{j,q})$ of order q associated with J equally spaced knots.

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We consider the following hierarchical prior on f

$$\Pi = \begin{cases} J \sim \Pi_J \\ a_1, \dots a_J \overset{iid}{\sim} \Pi_{a,J} \\ f(x) = J \sum_{j=1}^{J-1} (a_{j+1} - a_j) B_{j,q-1}(x). \end{cases}$$

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We then have

$$Kf(x) = \sum_{j=1}^{J} a_j B_{j,q}(x), \qquad \text{for } x \in [0,1],$$

and this prior is well suited for Hölder smooth functions.

Example 1: Numerical differentiation

Consider matrix Σ_n^q

$$(\Sigma_n^q)_{i,j} = \frac{1}{n} \sum_{l=1}^{n} B_{i,q}(x_l) B_{j,q}(x_l), \qquad i,j = 1, \dots, J.$$

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We require the following conditions on the design $x_1, x_2, \ldots, x_n$

- for all $v_1 \in \mathbb{R}^J$
$$J^{-1}\|v_1\|_J^2 \asymp v_1^T \Sigma_n^q v_1$$
- for all $v_2 \in \mathbb{R}^{J-1}$
$$(J-1)^{-1}\|v_2\|_{J-1}^2 \asymp v_2^T \Sigma_n^{(q-1)} v_2.$$

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These conditions are natural and satisfied by many designs, including the uniform design.

Example 1: Numerical differentiation

Theorem (K and Salomond, 201?)

Suppose the true f_0 is β-Hölder smooth, for $\beta \leq q-1$. Suppose that Π_J is such that for some constants $c_d, c_u > 0$ and $t \geq 0$,

$$\exp(-c_d j(\log j)^t) \leq \Pi_J(j \leq J \leq 2j), \qquad \Pi_J(J > j) \lesssim \exp(-c_u j(\log j)^t).$$

Suppose that for all $a_0 \in \mathbb{R}^J$, $\|a_0\|_\infty \leq H$, and some constant c

$$\Pi_{a,J}(\|a - a_0\|_J \leq \epsilon) \geq \exp(-cJ\log(1/\epsilon))$$

Then for some $C > 0$ and some $r > 0$

$$\mathrm{E}_0\Pi\Big(\|f - f_0\|_n \geq Cn^{-\frac{\beta}{3+2\beta}}(\log n)^{3r} \;\Big|\; Y\Big) \to 0.$$

Adaptive result, prior does not depend on β

Example 2: Deconvolution

For all $f \in L_2(\mathbb{R})$ define the operator K

$$Kf(x) = \int_{\mathbb{R}} f(t)\lambda(x-t)\,dt, \qquad \text{for } x \in \mathbb{R}$$

with the kernel $\lambda \in L_2(\mathbb{R})$ symmetric around 0.

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$$\Pi = \begin{cases} J \sim \Pi_J \\ v \sim \Pi_v \\ w_1, \ldots, w_J | J \sim \bigotimes_{j=1}^{J} N(0,1) \\ f(x) = \sum_{j=1}^{J} \frac{w_j}{\sqrt{2\pi v^2}} \exp\Big(-\frac{(x-z_j)^2}{2v^2} \Big) \end{cases}$$

with certain (tail) conditions on Π_j and Π_v, and the nodes $z_1, \ldots, z_J$

Example 2: Deconvolution

Theorem (K and Salomond, 201?)

Suppose the true f_0 is β-Sobolev smooth, for $\beta \in \mathbb{N}$, supported on $[0, 1]$. Suppose that the Fourier transform of the kernel λ satisfies

$$|\hat{\lambda}(t)| \asymp |t|^{-p}, \qquad \text{for } p \in \mathbb{N}.$$

Then for some $C > 0$ and some $r > 0$

$$\mathrm{E}_0 \Pi\Big(\|f - f_0\|_n \geq C n^{-\frac{\beta}{1+2\beta+2p}} (\log n)^r \;\Big|\; Y\Big) \to 0.$$

Adaptive result, prior does not depend on β

Example 3: extremely ill-posed and spectral cut-off

Recovery of the initial condition for the heat equation

The Dirichlet problem for the heat equation

$$\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}u(x,t), \quad u(x,0) = f(x), \quad u(0,t) = u(1,t) = 0,$$

where u is defined on $[0,1] \times [0,T]$ and the function $f \in L_2[0,1]$ satisfies $f(0) = f(1) = 0$

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The solution is given by

$$u(x,T) = \sqrt{2}\sum_i f_i e^{-i^2\pi^2 T}\sin(i\pi x) = \sum_i \kappa_i f_i e_i(x),$$

We observe a noisy version $u(\cdot\,,T)$, want to recover f

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Consider the extremely ill-posed problem

$$Y_i = \kappa_i f_i + \frac{1}{\sqrt{n}} Z_i,$$

where $\kappa_i \asymp \exp(-\gamma i^p)$ for some $\gamma > 0$ and $p \geq 1$.

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We take $\alpha \geq 0$ and $\xi > -2\gamma$, and consider the product prior

$$\Pi = \bigotimes_{i=1}^{k_n} N\big(0, i^{-\alpha} \exp(-\xi i^p)\big), \qquad k_n = \left(\frac{\log n}{\xi + 2\gamma} + O(\log\log n)\right)^{1/p}.$$

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$$k_n \text{ solves } 1 = n i^{-\alpha} \exp(-(\xi + 2\gamma) i^p)$$

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Theorem (K and Salomond, 201?)

Suppose the true f_0 is β-smooth. Then for every $M_n \to \infty$

$$E_0 \Pi\big(\|f - f_0\| \geq M_n (\log n)^{-\beta/p} \mid Y\big) \to 0.$$

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$K f_0$ is analytic and should be recovered at the rate $n^{-1/2}(\log n)^{1/(2p)}$, but the prior considered here leads to the following suboptimal rate

$$(\log n)^{-\frac{\beta}{p} + \frac{\gamma\alpha}{p(\xi+2\gamma)}} n^{-\frac{\gamma}{\xi+2\gamma}},$$

if $\xi > 0$.

Conclusions

Thank you for your attention!