A new way for achieving adaptation

ISBA-BNP Webinar

Sergios Agapiou (joint work with Ismael Castillo) 24th May 2023

Department of Mathematics and Statistics, University of Cyprus

- 1. Motivation
- 2. Setup
- 3. Contraction in the White Noise Model
- 4. General Results ρ -posteriors
- 5. Simulations
- 6. Conclusion

Motivation

• For (φ_k) an orthonormal basis of $L^2[0,1]$, let

$$f=\sum_{k=1}^{\infty}\sigma_k\zeta_k\varphi_k(\cdot),$$

where $\zeta_k \stackrel{iid}{\sim} h$ and $\sigma_k = \tau k^{-1/2-S}$, scaling $\tau > 0$, regularity S > 0.

• For (ψ_{lk}) an orthonormal wavelet basis of $L^2[0,1]$, let

$$f = \sum_{l=1}^{\infty} \sum_{k \in \mathcal{K}_l} s_l \zeta_{lk} \psi_{lk}(\cdot)$$

where $\zeta_{lk} \stackrel{iid}{\sim} h$ and $s_l = \tau 2^{-l(1/2+S)}$, scaling $\tau > 0$, regularity S > 0.

Literature - Rates of Contraction

- Gaussian: for appropriately tuned τ or S get minimax optimal contraction rates over Sobolev or Hölder regularity classes (not spatially inhomogeneous Besov)
 - A. van der Vaart and H. van Zanten, Rates of contraction of posterior distributions based on Gaussian process priors, Annals of Statistics, 2008
 - Many contributions in many settings!
- Laplace (more generally *p*-exponential): for appropriately tuned τ and/or *S* get minimax optimal contraction rates over Sobolev, Hölder, Besov classes
 - S. Agapiou, M. Dashti and T. Helin, Rates of contraction of posterior distributions based on p-exponential priors, Bernoulli, 2021
 - M. Giordano and K. Ray, Nonparametric Bayesian inference for reversible multidimensional diffusions, Annals of Statistics, 2022
 - S. Agapiou and S. Wang, Laplace priors and spatial inhomogeneity in Bayesian inverse problems, Bernoulli, 2023+
 - M. Giordano, Besov priors in density estimation: optimal posterior contraction rates and adaptation, arXiv:2208.14350
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Theorem (A., Dashti, Helin '21)

Assume $f_0 \in S^{\beta}$. Consider S-regular p-exponential priors $p \in [1, 2]$ with $\tau = 1$. Then the posterior contracts at rate

$$\epsilon_n = \begin{cases} n^{-\frac{\beta}{1+2\beta+\rho(S-\beta)}}, & \text{if } S > \beta\\ n^{-\frac{S}{1+2S}}, & \text{if } S \le \beta \end{cases}$$

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- If we could take p ≥ 0, for a fixed large S we would get the minimax rate without tuning for β ∈ (0, S)!
- If we could take $S \to \infty$, we would get the minimax rate for $\beta > 0!$

Setup

For (φ_k) orthonormal basis, (ψ_{lk}) orthonormal wavelet basis of $L^2[0,1]$

$$f = \sum_{k=1}^{\infty} \sigma_k \zeta_k \varphi_k(\cdot), \qquad f = \sum_{l=1}^{\infty} \sum_{k \in \mathcal{K}_l} s_l \zeta_{lk} \psi_{lk}(\cdot)$$

where

$$\sigma_k = k^{-1/2-S}$$
 or $\sigma_k = e^{-(\log k)^2}$

$$s_l = 2^{-l(1/2+S)}$$
 or $s_l = 2^{-l^2}$

We take i.i.d ζ 's from a heavy-tailed pdf h.

HT Assumptions

For some constants $c_1, c_2 > 0$ and $\kappa \ge 0$, assume

• *h* is symmetric, positive, bounded and decreasing on $[0,\infty)$

$$\log(1/h(x))\leq c_1(1+\log^{1+\kappa}(1+x)),\qquad x\geq 0$$

$$\overline{H}(x) := \int_x^\infty h(u) du \le \frac{c_2}{x^2}, \qquad x \ge 1$$

 $\kappa=$ 0: polynomial tails e.g. Cauchy or Student (for Cauchy $\overline{H}(x) symp x^{-1}$)

Heavy-tailed Priors in Applied BNP

- A. Shah, A. Wilson and Z. Ghahramani, Student-t Processes as Alternatives to Gaussian Processes, PMLR, 2014
- C. M. Carvalho, N. G. Polson, and J. G. Scott, *The horseshoe estimator for sparse signals*, Biometrika, 2010
- S. van der Pas, B. Szabo and A. van der Vaart, Uncertainty quantification for the horseshoe, Bayesian Analysis, 2017
- T. Sullivan, Well-posed Bayesian inverse problems and heavy-tailed stable quasi-Banach space priors, Inverse Problems and Imaging, 2017
- M. Markkanen, L. Roininen, J. Huttunen and S. Lasanen, Cauchy difference priors for edge-preserving Bayesian inversion, Journal of Inverse and III-posed Problems, 2019
- J. Suuronen, N. Chada and L. Roininen, Cauchy Markov Random Field Priors for Bayesian Inversion, Statistics and Computing, 2022

Regularity Assumptions for the Truth

We will consider three types of smoothness assumptions:

• Sobolev: $f_0 \in \mathcal{S}(\beta, L)$ for some $\beta, L > 0$ if

$$\sum_{k=1}^{\infty} k^{2\beta} f_{0,k}^2 \leq L^2.$$

• Hölder (Zygmund): $f_0 \in \mathcal{H}(\beta, L)$ for some $\beta, L > 0$ if

$$2^{l(1/2+\beta)} \max_{k \in \mathcal{K}_l} |f_{0,lk}| \le L.$$

• Besov: $f_0 \in \mathcal{B}(\beta, r, L)$, for some $\beta > 0$, $1 \le r \le 2$, L > 0 if

$$\sum_{l=1}^{\infty} 2^{rl(\beta+1/2-1/r)} \sum_{k \in \mathcal{K}_l} |f_{lk}|^r \le L^r.$$

For r < 2 spatial inhomogeneity

Contraction in the White Noise Model

• Equivalently consider the normal sequence model

 $X_k | f_k \sim \mathcal{N}(f_k, 1/n)$ (single index)

or

$$X_{lk}|f_{lk} \sim \mathcal{N}(f_{lk}, 1/n)$$
 (double index)

• We denote by $X^{(n)}$ the corresponding observation sequence.

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Moment Assumption

$$\int_{-\infty}^{\infty} x^2 h(x) dx < \infty \quad \text{or} \quad \int_{-\infty}^{\infty} |x|^q h(x) dx < \infty, \ q \ge 1$$

Theorem (A and Castillo '23+)

Let Π be a heavy-tailed series prior defined via an orthonormal basis (φ_k) , for *h* satisfying the *HT* Assumptions and the Moment Assumption with q = 2.

Let $f_0 \in \mathcal{S}(\beta, L)$ for L > 0 and consider one of the next two settings:

•
$$\sigma_k = k^{-1/2-S}$$
 for $S \ge \beta$;

•
$$\sigma_k = e^{-(\log k)^2}, \ \beta > 0.$$

Then in either setting, as $n \to \infty$

$$E_{f_0}\left[\int \|f-f_0\|_2^2 d\Pi(f\,|\,X)\right] \lesssim n^{-\frac{2\beta}{2\beta+1}} (\log n)^d$$

for some d > 0.

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•
$$s_l = 2^{-l(1/2+S)}$$
 for $S > \{(1/q + \frac{\beta}{1+2\beta}) \lor \beta\};$

•
$$s_l = 2^{-l^2}, \ \beta > 0.$$

Then in either setting, as $n o \infty$

$$E_{f_0}\left[\int \|f-f_0\|_{\infty}d\Pi(f\mid X)
ight]\lesssim (n/\log n)^{-rac{eta}{2eta+1}}(\log n)^d,$$

for some d > 0.

Corollary

By Markov inequality, the two last results imply in their corresponding settings that as $n \to \infty$

$$E_{f_0}\Pi[\{f: \|f-f_0\|_2 > \mathcal{L}_n n^{-\frac{\beta}{2\beta+1}}\} | X^{(n)}] \to 0,$$

and

$$E_{f_0}\Pi[\{f: \|f-f_0\|_{\infty} > \mathcal{L}_n(n/\log n)^{-\frac{\beta}{2\beta+1}}\} | X^{(n)}] \to 0,$$

respectively, where $\mathcal{L}_n = (\log n)^d$ for some d > 0.

- L2-loss with $\sigma_k = k^{-1/2-S}$ and $|f_{0,k}| \lesssim k^{-1/2-eta}$, other cases similar
- Need to bound

$$E_{f_0}\left[\int \|f-f_0\|_2^2 d\Pi(f \mid X)\right],$$

work coefficient-wise

- L₂-loss with $\sigma_k = k^{-1/2-S}$ and $|f_{0,k}| \lesssim k^{-1/2-\beta}$, other cases similar
- Need to bound

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Using heavy tails assumption

$$E_{f_0}\int (f_k-f_{0,k})^2d\Pi(f\mid X)\lesssim n^{-1}\log^{1+\kappa}\left(1+rac{L+1/\sqrt{n}}{\sigma_k}
ight)$$

• For $k \leq K_n := n^{1/(1+2\beta)}$, since $\sigma_k^{-1} \leq \sigma_{K_n}^{-1}$, bound logarithmic in n!

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• For $k \leq K_n := n^{1/(1+2\beta)}$, since $\sigma_k^{-1} \leq \sigma_{K_n}^{-1}$, bound logarithmic in n!

• The total contribution to the error of all $k \leq K_n$, for any S > 0, is

$$\lesssim n^{-1} (\log n)^d K_n \lesssim n^{-rac{2eta}{1+2eta}} (\log n)^d$$

- L2-loss with $\sigma_k = k^{-1/2-S}$ and $|f_{0,k}| \lesssim k^{-1/2-eta}$, other cases similar
- Need to bound $E_{f_0}\left[\int \|f-f_0\|_2^2d\Pi(f\,|\,X)\right],$

work coefficient-wise

- For $k > K_n$ use $(f_k f_{0,k})^2 \le 2f_k^2 + 2f_{0,k}^2$
 - Assumption on f_0 implies 2nd term is small
 - Oversmoothing prior suggests 1st term also small under the posterior
 - Delicate analysis shows that for $S \ge \beta$ the contribution to the squared error is also $n^{-\frac{2\beta}{1+2\beta}}(\log n)^d$

Behaviour of Student Prior

- $X \sim \mathcal{N}(f, 10^{-5})$
- $f\sim\sigma t_3$
- $\sigma = 20^{-5.5}$ (left) and $\sigma = (2e9)^{-5.5}$ (right) (S = 5)



Behaviour of Student Prior

$$\sigma = 20^{-5.5}$$
 (blue) and $\sigma = (2e9)^{-5.5}$ (red dashed)



Behaviour of Student Prior

$$\sigma = 20^{-5.5}$$
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Similar to spike and slab prior I. Johnstone and B. Silverman, Annals of Statistics, 2004, 2005

Contraction in White Noise Model - Besov truth

- Besov spaces \mathcal{B}_{rr}^{β} with $1 \leq r < 2$ model spatial inhomogeneity
- Allow for large wavelet coefficients in high frequencies
- Gaussian priors are limited by the linear minimax rate $n^{-\frac{\beta+1/2-1/r}{2+2\beta-2/r}}$
 - S. Agapiou and S. Wang, Laplace priors and spatial inhomogeneity in Bayesian inverse problems, Bernoulli, 2023+
- Laplace priors can achieve the minimax rate (r = 1) or nearly the minimax rate (r > 1), but require tuning both S and τ
 - S. Agapiou, M. Dashti and T. Helin, Rates of contraction of posterior distributions based on p-exponential priors, Bernoulli, 2021
 - S. Agapiou and A. Savva, Adaptive inference over Besov spaces in the white noise model using p-exponential priors, arXiv:2209.06045

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Let
$$f_0 \in \mathcal{B}(\beta, r, L)$$
 for $1 \le r \le 2, L > 0$ and $\beta > 1/r - 1/2$.
Then for $s_l = 2^{-l^2}$, as $n \to \infty$

$$E_{f_0}\left[\int \|f-f_0\|_2^2 d\Pi(f\,|\,X)\right] \lesssim n^{-\frac{2\beta}{2\beta+1}} (\log n)^d,$$

for some d > 0.

General Results - ρ -posteriors

Theorem (A and Castillo '23+)

Let Π be a heavy-tailed series prior defined via an orthonormal basis (φ_k) , for *h* satisfying the *HT* Assumptions.

Let $f_0 \in \mathcal{S}(\beta, L)$ for L > 0 and consider one of the next two settings:

•
$$\sigma_k = k^{-1/2-S}$$
 for $S > 1/2$, $\beta \le S$;

•
$$\sigma_k = e^{-(\log k)^2}, \ \beta > 0.$$

In either setting there exist $c_1, c_2, d > 0$ such that

$$\Pi[\|f - f_0\|_2 < c_1\varepsilon_n] \ge e^{-c_2n\varepsilon_n^2},$$

with

$$\varepsilon_n = (\log n)^d n^{-\frac{\beta}{1+2\beta}}.$$

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Let $f_0 \in \mathcal{H}(\beta, L)$ for L > 0 and consider one of the next two settings:

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$$s_l = 2^{-l(1/2+S)}$$
 for $S > 1/2$, $\beta \le S_s$

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In either setting there exist $c_1, c_2, d > 0$ such that

$$\Pi[\|f-f_0\|_{\infty} < c_1\varepsilon_n] \ge e^{-c_2n\varepsilon_n^2},$$

with

$$\varepsilon_n = (\log n)^d n^{-\frac{\beta}{2\beta+1}}.$$

Generic Prior Mass Condition - Proof Ideas

- Focus on L_2 -loss with $\sigma_k = k^{-1/2-S}$ and $f_0 \in S(\beta, L)$, other cases similar
- For some K to be chosen, split to low and high frequencies

$$\Pi[\|f - f_0\|_2 < \varepsilon] \ge \Pi \left[\|f^{[K]} - f_0^{[K]}\|_2 < \varepsilon/2 \right] \Pi \left[\|f^{[K^c]} - f_0^{[K^c]}\|_2 < \varepsilon/2 \right]$$

- For some *K* to be chosen, split to low and high frequencies $\Pi[\|f - f_0\|_2 < \varepsilon] \ge \Pi \left[\|f^{[K]} - f_0^{[K]}\|_2 < \varepsilon/2 \right] \Pi \left[\|f^{[K^c]} - f_0^{[K^c]}\|_2 < \varepsilon/2 \right]$
- f₀ ∈ S(β; L) implies even for small k the coefficients f_{0,k} cannot be too large and so prior puts substantial mass around them
- Since h is heavy tailed, even if σ_k decays very quickly (oversmoothing prior), this mass is still substantial!

$$\begin{aligned} \Pi \left[\| f^{[K]} - f_0^{[K]} \|_2 &< \varepsilon/2 \right] &\geq \varepsilon^K \exp\{ -C_1 K \log^{1+\kappa} (C_2 / \sigma_K) \} \\ &\geq \varepsilon^K \exp\{ -C_1' K \log^{1+\kappa} K \} \end{aligned}$$

• For some ${\boldsymbol{K}}$ to be chosen, split to low and high frequencies

$$\Pi[\|f - f_0\|_2 < \varepsilon] \ge \Pi \left[\|f^{[K]} - f_0^{[K]}\|_2 < \varepsilon/2 \right] \Pi \left[\|f^{[K^c]} - f_0^{[K^c]}\|_2 < \varepsilon/2 \right]$$

$$\Pi\left[\|f^{[K^c]} - f_0^{[K^c]}\|_2 < \varepsilon/2\right] \ge \Pi\left[\|f^{[K^c]}\|_2 < \varepsilon/4\right] \, \mathbb{1}_{\|f_0^{[K^c]}\|_2 < \varepsilon/4}$$

- $f_0 \in \mathcal{S}(\beta; L)$ implies $\|f_0^{[K^c]}\|_2$ is small for large K
- For S large enough and $\varepsilon \asymp K^{-\beta} \log K$

$$\Pi\left[\|f^{[K^c]}\|_2 < \varepsilon/4\right] \ge \exp(-C_3 K)$$

• For some K to be chosen, split to low and high frequencies

 $\Pi[\|f - f_0\|_2 < \varepsilon] \ge \Pi \left[\|f^{[K]} - f_0^{[K]}\|_2 < \varepsilon/2 \right] \, \Pi \left[\|f^{[K^c]} - f_0^{[K^c]}\|_2 < \varepsilon/2 \right]$

• Combining, for large K and $\varepsilon \simeq K^{-\beta} \log K$ it holds

$$\Pi[\|f - f_0\|_2 < \varepsilon] \ge \exp\{-CK \log^{1+\kappa} K\}$$

Optimize choice K = K(n) so that ε ≍ K^{-β} log K as small as possible while K log^{1+κ} K ≍ nε²

Contraction Results for *p***-posteriors**

- Both results can be extended to cover Cauchy priors (*H*(x) ≍ x⁻¹), provided S > 1 for the S-regular cases.
- Combining with Theorem 8.43 of GV17, these prior mass conditions imply contraction results for pseudo-posteriors

$$\Pi^{(\rho)}(\theta \in B|X) = \frac{\int_B p_\theta^{\rho}(X) d\Pi_n(\theta)}{\int p_\theta^{\rho}(X) d\Pi_n(\theta)}, \quad \rho \in (0,1).$$

• Example 8.44 of GV17 shows that for i.i.d observations, under the prior mass condition $\Pi(\theta : K(p_{f_0}; p_f) < \varepsilon_n^2) \ge \exp(-n\varepsilon_n^2)$, we have

$$\Pi_n^{(\rho)}(d_H(p_{f_0},p_f)>M_n\varepsilon_n\,|\,X_1,\ldots,X_n)\to 0,$$

for any $M_n \to \infty$.

S. Ghoshal and A. vd Vaart, Fundamentals of nonparametric Bayesian inference, 2017.

Contraction Results for ρ -posteriors

• e.g. density estimation with

$$p_f(x) = \frac{e^{f(x)}}{\int e^{f(x)} dx}$$

and a prior on f

• Lemma 2.5 of GV17 shows

$$K(p_f; p_g) \lesssim \|f - g\|_{\infty}^2 e^{\|f - g\|_{\infty}} (1 + \|f - g\|_{\infty})$$

- The prior mass condition in L[∞]-loss suffices for showing contraction of ρ-posteriors in Hellinger distance at the nearly minimax rate ε_n over Hölder smoothness
- Partial adaptivity $s_l = 2^{-(1/2+S)l}$ / adaptivity $s_l = 2^{-l^2}$ (up to logs)

Simulations

White Noise Model - Sobolev Truth

- Study linear inverse problem in simulations of
 B. Knapik, B. Szabo, A. van der Vaart and H. Zanten, Bayes procedures for adaptive inference in inverse problems for the white noise model, PTRF, 2016
- Equivalent to normal sequence model

$$X_k \sim \mathcal{N}(\lambda_k f_k, 1/n)$$

defined wrt the eigenbasis of the forward operator

$$arphi_k(t)=\sqrt{2}\cos(\pi(k-1/2)t),t\in[0,1]$$

where

$$\lambda_k = \pi/(k-1/2)$$

are the corresponding eigenvalues

• Coefficients of truth

$$f_{0,k} = k^{-3/2} \sin(k)$$

"Sobolev regularity $\beta = 1$ "

• Priors

- Gaussian hierarchical regularity prior:

$$f_k|S \sim \mathcal{N}(0,\sigma_k^2), \quad \sigma_k = k^{-1/2-S}, \quad S \sim \textit{Exp}(1)$$

- Student t_3 oversmoothing prior 1: $\sigma_k = k^{-1/2-5}, \ S = 5$

- Student t_3 oversmoothing prior 2: $\sigma_k = e^{-(\log k)^{3/2}}$

- Truncate up to k = 200
- Gaussian hierarchical: use non-centered Gibbs sampler
- Student: product of univariate problems, use RW Metropolis on each

White Noise Model - Sobolev Truth - Full Posteriors



White Noise Model - Sobolev Truth - ρ -posteriors

Student t_3 , decay 2

 $n = 10^{5}$



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White Noise Model - NMR Signal

- Denoising (no inversion) NMR signal
- Expand in Symmlet 6 wavelet basis (ψ_{lk}) truncated at l = 9

$$X_{lk} \sim \mathcal{N}(f_{lk}, 1/n)$$

• Student t_3 oversmoothing prior on f_{lk} with

$$s_l = 2^{-l^{3/2}}, \ \forall k \in \mathcal{K}_l$$

 Product of univariate problems, use RW Metropolis to sample each posterior



J. Buckheit, S. Chen, D. Donoho, I. Johnstone, and J. Scargle, Wavelab 850

White Noise Model - NMR Signal



White Noise Model - NMR Signal



•
$$X^{(n)} = (X_1, \dots, X_n)$$
 where $X_j \stackrel{iid}{\sim} p(x), x \in [0, 1]$

• $p: [0,1] \rightarrow R^+$ unknown density, modelled as

$$p(x) = \frac{e^{f(x)}}{\int e^{f(x)} dx}$$

• True density *p*₀ defined via *f*₀, which has coefficients wrt Symmlet 8 wavelet basis

$$f_{0,lk} = 4\cos^3(2^l + k)2^{-(5/2)l}$$

Hölder-Zygmund regularity $\beta = 2$

- Wavelet priors on f
 - Gaussian oversmoothing prior: $\textit{s}_{\textit{l}}=2^{-(1/2+\textit{S})\textit{l}},~\textit{S}=5$
 - Cauchy oversmoothing prior 1: $s_l = 2^{-(1/2+S)l}, S = 5$
 - Cauchy oversmoothing prior 2: $s_l = 2^{-l^{3/2}}$
- Sampled posterior using Whitened Precondition Crank-Nicolson algorithm, based on orthogonal transformation for Cauchy

V. Chen, M. Dunlop, O. Papaspiliopoulos and A. Stuart, Dimension robust MCMC in Bayesian inverse problems, arXiv:1803.03344

Density Estimation - Full Posteriors



Density Estimation - ρ -posteriors



Conclusion

Outlook

Summary:

- Adaptivity with minimal/no tuning with heavy tailed priors
- Posterior contraction results for WNM
- $\bullet\,$ Generic prior mass condition can give $\rho\text{-posterior}$ contraction results for general models
- Results in L^2 and L^∞ losses, for Sobolev, Hölder and Besov truths
- Promising simulations, despite multimodal posteriors

Still to do:

- Uncertainty quantification
- Inverse problems
- Posterior contraction for general models
- Computation

Thank you!