



Weierstraß-Institut für
Angewandte Analysis und Stochastik



Bayesian inference and stochastic optimization

Vladimir Spokoiny ,
WIAS, HU Berlin

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Let $\mathbf{Y}$ denote the observed random data, $\mathbf{Y} \sim \mathbb{P}$. A general **parametric approach (PA)**: $\mathbb{P} \in (\mathbb{P}_{\boldsymbol{\theta}}, \boldsymbol{\theta} \in \Theta \subseteq \mathbb{R}^{\infty})$.

The **log-likelihood** function

$$L(\boldsymbol{\theta}) = L(\mathbf{Y}, \boldsymbol{\theta}) \stackrel{\text{def}}{=} \log \frac{d\mathbb{P}_{\boldsymbol{\theta}}}{d\boldsymbol{\mu}_0}(\mathbf{Y}).$$

MLE of $\boldsymbol{\theta}$ by maximizing the function $L(\boldsymbol{\theta})$:

$$\tilde{\boldsymbol{\theta}} \stackrel{\text{def}}{=} \operatorname{argmax}_{\boldsymbol{\theta} \in \Theta} L(\boldsymbol{\theta}).$$

Target (the best parametric fit):

$$\boldsymbol{\theta}^* \stackrel{\text{def}}{=} \operatorname{argmax}_{\boldsymbol{\theta} \in \Theta} \mathbb{E} L(\boldsymbol{\theta}).$$

In the **Bayes setup** ϑ is a random element, $\vartheta \sim \Pi$ on the parameter set Θ , **a prior**.

The **posterior** describes the conditional distribution of ϑ given $\mathbf{Y}$

$$\vartheta \mid \mathbf{Y} \propto \exp\{L(\boldsymbol{\theta})\} \Pi(d\boldsymbol{\theta}).$$

A Gaussian prior $\Pi \sim \mathcal{N}(0, G^{-2})$ yields

$$\vartheta \mid \mathbf{Y} \propto \exp\{L_G(\boldsymbol{\theta})\},$$

$$L_G(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) - \|G\boldsymbol{\theta}\|^2/2.$$

Prior Π induces a **penalty** $-\log \Pi(\boldsymbol{\theta})$ leading to penalized MLE

$$\tilde{\boldsymbol{\theta}}_{\Pi} = \operatorname{argmax}_{\boldsymbol{\theta}} L_{\Pi}(\boldsymbol{\theta}) = \operatorname{argmax}_{\boldsymbol{\theta}} \{L_{\Pi}(\boldsymbol{\theta}) - \log \Pi(\boldsymbol{\theta})\}.$$

Gaussian priors lead to **quadratic penalization**

$$\tilde{\boldsymbol{\theta}}_G = \operatorname{argmax}_{\boldsymbol{\theta}} L_G(\boldsymbol{\theta}) = \operatorname{argmax}_{\boldsymbol{\theta}} \{L_G(\boldsymbol{\theta}) - \|G\boldsymbol{\theta}\|^2/2\}.$$

Posterior $\boldsymbol{\vartheta}_G \mid \mathbf{Y}$ is a random measure with the density

$$\boldsymbol{\vartheta}_G \mid \mathbf{Y} \propto \exp L_G(\boldsymbol{\theta})$$

Formally, Bayes approach replaces the **max** of L_G by the **soft-max**.

■ Posterior mean and MAP

$$\tilde{\boldsymbol{\theta}}_{\text{MAP}} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \exp L_G(\boldsymbol{\theta}) = \tilde{\boldsymbol{\theta}}_G$$

$$\bar{\boldsymbol{\theta}}_G \stackrel{\text{def}}{=} \frac{\int \boldsymbol{\theta} \exp L_G(\boldsymbol{\theta}) d\boldsymbol{\theta}}{\int \exp L_G(\boldsymbol{\theta}) d\boldsymbol{\theta}};$$

■ Concentration (contraction) set $\mathcal{A}$:

$$\rho(\mathcal{A}) \stackrel{\text{def}}{=} \frac{\int_{\mathcal{A}^c} \exp L_G(\boldsymbol{\theta}) d\boldsymbol{\theta}}{\int_{\mathcal{A}} \exp L_G(\boldsymbol{\theta}) d\boldsymbol{\theta}}$$

■ Credible sets $\mathcal{A}(\alpha)$

$$IP(\boldsymbol{\vartheta}_G \in \mathcal{A}(\alpha) \mid \mathbf{Y}) = 1 - \alpha;$$

■ Elliptic credible sets $\mathcal{A}_G(\alpha) = \{\boldsymbol{\theta} : \|D(\boldsymbol{\vartheta}_G - \tilde{\boldsymbol{\theta}}_G)\| \leq z_\alpha\}.$

$$\tilde{\boldsymbol{\theta}}_G = \operatorname{argmax}_{\boldsymbol{\theta}} L_G(\boldsymbol{\theta}), \quad \boldsymbol{\theta}_G^* = \operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E} L_G(\boldsymbol{\theta})$$

■ Elliptic concentration sets around $\boldsymbol{\theta}_G^*$:

$$\mathbb{P}(\|D_G(\tilde{\boldsymbol{\theta}}_G - \boldsymbol{\theta}_G^*)\| > \mathbf{r}_G(\mathbf{x})) \leq e^{-\mathbf{x}},$$

where

$$D_G^2 = -\nabla^2 \mathbb{E} L_G(\boldsymbol{\theta}_G^*),$$

$$\mathbf{r}_G(\mathbf{x}) \approx \sqrt{\mathbf{p}_G} + \sqrt{2\mathbf{x}},$$

$$\mathbf{p}_G = \operatorname{tr}(D_G^{-2} \operatorname{Var}(\nabla L_G(\boldsymbol{\theta}_G^*))).$$

■ Fisher expansion

$$\|D_G(\tilde{\boldsymbol{\theta}}_G - \boldsymbol{\theta}_G^*) - D_G^{-1} \nabla L_G(\boldsymbol{\theta}_G^*)\| \leq 3\mathbf{r}_G^{-1} \delta_{3,G}(\mathbf{r}_G).$$

Contraction sets $\mathcal{A}$: for $x > 0$ build $\mathcal{A}$ s.t.

$$\rho(\mathcal{A}) \stackrel{\text{def}}{=} \frac{\int_{\mathcal{A}^c} \exp\{L_G(\boldsymbol{\theta})\} d\boldsymbol{\theta}}{\int_{\mathcal{A}} \exp\{L_G(\boldsymbol{\theta})\} d\boldsymbol{\theta}} \leq e^{-x} \quad \text{whp}$$

in the form

$$\mathcal{A} = \tilde{\mathcal{A}}(r_0) = \{\boldsymbol{\theta} : \|\tilde{D}(\boldsymbol{\theta} - \tilde{\boldsymbol{\theta}}_G)\| \leq r_0\},$$

Gaussian approximation:

$$\sup_{A \in \mathcal{B}_s(\mathbb{R}^p)} \left| IP(\boldsymbol{\vartheta}_G - \tilde{\boldsymbol{\theta}}_G \in A \mid \mathbf{Y}) - IP'(\tilde{D}_G^{-1}\boldsymbol{\gamma} \in A) \right| \lesssim \frac{p_G + x}{n}$$

$$\sup_{A \in \mathcal{B}(\mathbb{R}^p)} \left| IP(\boldsymbol{\vartheta}_G - \tilde{\boldsymbol{\theta}}_G \in A \mid \mathbf{Y}) - IP'(\tilde{D}_G^{-1}\boldsymbol{\gamma} \in A) \right| \lesssim \frac{(p_G + x)^{3/2}}{n^{1/2}}$$

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- Log-likelihood $L(\boldsymbol{\theta}) = L(\mathbf{Y}, \boldsymbol{\theta})$.
- Prior Π and penalized log-likelihood

$$L_{\Pi}(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) + \log \Pi(\boldsymbol{\theta})$$

- Gaussian prior $\mathcal{N}(0, G^{-2})$ and quadratic penalization

$$L_G(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) - \|G\boldsymbol{\theta}\|^2/2$$

- Penalized MLE

$$\tilde{\boldsymbol{\theta}}_G = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} L_G(\boldsymbol{\theta})$$

- Posterior $\boldsymbol{\vartheta} \mid \mathbf{Y}$

$$\boldsymbol{\vartheta} \mid \mathbf{Y} \propto \exp L_G(\boldsymbol{\theta})$$

True value

$$\boldsymbol{\theta}^* = \operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E} L(\boldsymbol{\theta}).$$

- The penalized MLE $\tilde{\boldsymbol{\theta}}_G$ concentrates around

$$\boldsymbol{\theta}_G^* = \operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E} L_G(\boldsymbol{\theta})$$

yielding the **bias** $\boldsymbol{\theta}_G^* - \boldsymbol{\theta}^*$.

- The posterior measure $\vartheta \mid \mathbf{Y}$ concentrates around $\tilde{\boldsymbol{\theta}}_G$
- $\vartheta \mid \mathbf{Y}$ is nearly Gaussian.

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(E) *The stochastic component $\zeta(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) - \mathbb{E}L(\boldsymbol{\theta})$ of the process $L(\boldsymbol{\theta})$ is linear in $\boldsymbol{\theta}$:*

$$\nabla \zeta \equiv \nabla \zeta(\boldsymbol{\theta}).$$

(ED₀) *There exist a positive symmetric matrix V , and constants $g > 0$, $\nu_0 \geq 1$ such that $\text{Var}(\nabla \zeta) \leq V^2$ and*

$$\sup_{\mathbf{u} \in \mathbb{R}^p} \log \mathbb{E} \exp \left\{ \lambda \frac{\langle \mathbf{u}, \nabla \zeta \rangle}{\|V \mathbf{u}\|} \right\} \leq \frac{\nu_0^2 \lambda^2}{2}, \quad |\lambda| \leq g.$$

($\mathcal{L}$) The set Θ is open and convex in $\mathbb{R}^p$. The function $\mathbb{E}L(\boldsymbol{\theta})$ is concave in $\boldsymbol{\theta} \in \Theta$.

Define for each $\boldsymbol{\theta} \in \Theta^\circ$, and any $\mathbf{u} \in \mathbb{R}^p$, the directional derivative

$$\delta_m(\boldsymbol{\theta}, \mathbf{u}) \stackrel{\text{def}}{=} \frac{1}{m!} \frac{d^m}{dt^m} \mathbb{E}L(\boldsymbol{\theta} + t\mathbf{u}) \Big|_{t=0}, \quad m = 3, 4.$$

($\mathcal{L}_0$) The functions $\delta_3(\boldsymbol{\theta}, \mathbf{u})$ and $\delta_4(\boldsymbol{\theta}, \mathbf{u})$ are well defined and uniformly bounded for all $\boldsymbol{\theta} \in \Theta^\circ$ and all $\mathbf{u} \in \mathcal{U}$ for specific sets Θ° and $\mathcal{U}$ in $\mathbb{R}^p$.

Clearly the value $\delta_3(\boldsymbol{\theta}, \mathbf{u})$ is proportional to $\|\mathbf{u}\|^3$, while $\delta_4(\boldsymbol{\theta}, \mathbf{u}) \asymp \|\mathbf{u}\|^4$.

Define

$$D^2(\boldsymbol{\theta}) = -\nabla^2 \mathbb{E} L(\boldsymbol{\theta}), \quad D_G^2 = D^2(\boldsymbol{\theta}) + G^2.$$

(V|G) Signal-noise:

$$B_{V|G}(\boldsymbol{\theta}) \stackrel{\text{def}}{=} D_G^{-1}(\boldsymbol{\theta}) V^2 D_G^{-1}(\boldsymbol{\theta})$$

with V^2 from $(\mathbf{E}D_0)$. There are fixed constants $\lambda_{V|G}$ and $p_{V|G}$ such that

$$\text{tr } B_{V|G}(\boldsymbol{\theta}) \leq p_{V|G}, \quad \|B_{V|G}\| \leq \lambda_{V|G}, \quad \boldsymbol{\theta} \in \Theta^\circ.$$

(D|G) The local effective dimension: for a fixed constant C

$$p_G(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \text{tr} \{ D^2(\boldsymbol{\theta}) D_G^{-2}(\boldsymbol{\theta}) \} \leq C, \quad \boldsymbol{\theta} \in \Theta^\circ.$$

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By (E) , the stochastic component $\zeta(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) - \mathbb{E}L(\boldsymbol{\theta})$ is linear in $\boldsymbol{\theta}$ and $\nabla\zeta = \nabla\zeta(\boldsymbol{\theta})$ does not depend on $\boldsymbol{\theta}$.

Theorem

Under condition (ED_0) , there exists a random set $\Omega(\mathbf{x})$ with $\mathbb{P}(\Omega(\mathbf{x})) \geq 1 - Ce^{-x}$ such that on this set

$$\|D_G^{-1}\nabla\zeta\| \leq z(B_{V|G}, \mathbf{x}),$$

where $B_{V|G} = D_G^{-1}V^2D_G^{-1}$ and

$$z(B_{V|G}, \mathbf{x}) = \sqrt{\text{tr } B_{V|G}} + \sqrt{2x\lambda_{\max}(B_{V|G})}.$$

Let $\theta_G^* = \operatorname{arginf}_{\theta} \mathbb{E} L_G(\theta)$ and $D_G^2 = D^2(\theta_G^*) + G^2$.

Theorem

Let $\|D_G^{-1} \nabla \zeta\| \leq z(B_{V|G}, \mathbf{x})$ on a random set $\Omega(\mathbf{x})$ with $\mathbb{P}(\Omega(\mathbf{x})) \geq 1 - e^{-x}$. Let

$$\mathcal{A}_G(\mathbf{r}_G) \stackrel{\text{def}}{=} \{\theta: \|D_G(\theta - \theta_G^*)\| \leq \mathbf{r}_G\}$$

$$(1 - \rho)\mathbf{r}_G \geq z(B_{V|G}, \mathbf{x}).$$

Then on $\Omega(\mathbf{x})$

$$\|D_G(\tilde{\theta}_G - \theta_G^*)\| \leq \mathbf{r}_G.$$

Local set

$$\mathcal{A}_G(\mathbf{r}_G) \stackrel{\text{def}}{=} \{\boldsymbol{\theta}: \|D_G(\boldsymbol{\theta} - \boldsymbol{\theta}_G^*)\| \leq \mathbf{r}_G\}.$$

Use **local smoothness** of $-\mathbb{E}L_G(\boldsymbol{\theta})$ to show that for $\boldsymbol{\theta} \in \mathcal{A}_G(\mathbf{r}_G)$

$$\begin{aligned} -\{\mathbb{E}L_G(\boldsymbol{\theta}) - \mathbb{E}L_G(\boldsymbol{\theta}_G^*)\} &\approx \|D_G(\boldsymbol{\theta} - \boldsymbol{\theta}_G^*)\|^2/2, \\ -\nabla \mathbb{E}L_G(\boldsymbol{\theta}) &\approx D_G^2(\boldsymbol{\theta} - \boldsymbol{\theta}_G^*) \end{aligned}$$

Use **convexity** of $\mathbb{E}L_G(\boldsymbol{\theta})$ to show that

$$\|\nabla \mathbb{E}L_G(\boldsymbol{\theta})\| \geq \mathbf{r}_G, \quad \boldsymbol{\theta} \notin \mathcal{A}_G(\mathbf{r}_G).$$

Use $\|D_G^{-1}\nabla\zeta\| \leq z(B_{V|G}, \mathbf{x})$ to show

$$\nabla L(\boldsymbol{\theta}) = \nabla \mathbb{E}L(\boldsymbol{\theta}) + \nabla\zeta \neq 0, \quad \boldsymbol{\theta} \notin \mathcal{A}_G(\mathbf{r}_G).$$

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Concentration sets of the posterior in nonparametric models using

- Empirical process theory, large deviations of the log-likelihood and covering numbers and chaining arguments
- small ball probability
- local smoothness

See e.g.

- Ghoshal, S., Ghosh, J. K., van der Vaart, A. W. (2000) Convergence rates of posterior distributions. Ann.Statist., 28, 500–531.
- van der Vaart, A. W., van Zanten, J. H. (2008) Rates of contraction of posterior distributions based on Gaussian process priors. Ann. Statist., 36, 1031–1508.

Concentration set of $\vartheta_G - \tilde{\theta}_G$ | Y contraction

Define the elliptic set $\tilde{\mathcal{A}}(\mathbf{r}_0) = \{\mathbf{u}: \|\tilde{D}\mathbf{u}\| \leq \mathbf{r}_0\}$ with $\tilde{D}^2 = D^2(\tilde{\theta}_G)$. Consider the random quantity

$$\rho(\mathbf{r}_0) \stackrel{\text{def}}{=} \frac{\int_{\tilde{\mathcal{A}}(\mathbf{r}_0)^c} \exp\{L_G(\tilde{\theta}_G + \mathbf{u})\} d\mathbf{u}}{\int_{\tilde{\mathcal{A}}(\mathbf{r}_0)} \exp\{L_G(\tilde{\theta}_G + \mathbf{u})\} d\mathbf{u}}.$$

Theorem

Let, for some fixed values $\mathbf{r}_0$ and $\mathbf{x} > 0$, it hold

$$C_0 \mathbf{r}_0 \geq 2\sqrt{p_G(\boldsymbol{\theta})} + \sqrt{\mathbf{x}}, \quad \boldsymbol{\theta} \in \Theta^\circ.$$

Then, on the random set $\Omega(\mathbf{x})$ from Theorem 2, with $\tilde{p}_G = p_G(\tilde{\theta}_G)$

$$\rho(\mathbf{r}_0) \leq \exp\{-(\tilde{p}_G + \mathbf{x})/2\}.$$

Let $\tilde{\boldsymbol{\theta}}_G = \operatorname{arginf}_{\boldsymbol{\theta}} L_G(\boldsymbol{\theta})$. The use of $\nabla L_G(\tilde{\boldsymbol{\theta}}_G) = 0$ allows to represent

$$\begin{aligned}\rho(\mathbf{r}_0) &= \frac{\int_{\|\tilde{D}\mathbf{u}\| > \mathbf{r}_0} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u}) - L_G(\tilde{\boldsymbol{\theta}}_G)\} d\mathbf{u}}{\int_{\|\tilde{D}\mathbf{u}\| \leq \mathbf{r}_0} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u}) - L_G(\tilde{\boldsymbol{\theta}}_G)\} d\mathbf{u}} \\ &= \frac{\int_{\|\tilde{D}\mathbf{u}\| > \mathbf{r}_0} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u}) - L_G(\tilde{\boldsymbol{\theta}}_G) - \langle \nabla L_G(\tilde{\boldsymbol{\theta}}_G), \mathbf{u} \rangle\} d\mathbf{u}}{\int_{\|\tilde{D}\mathbf{u}\| \leq \mathbf{r}_0} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u}) - L_G(\tilde{\boldsymbol{\theta}}_G) - \langle \nabla L_G(\tilde{\boldsymbol{\theta}}_G), \mathbf{u} \rangle\} d\mathbf{u}}.\end{aligned}$$

Fix $\boldsymbol{\theta} \in \mathcal{A}_G(\mathbf{r}_G)$. Consider $f(\boldsymbol{\theta}) = \mathbb{E} L_G(\boldsymbol{\theta})$. As $\zeta(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) - \mathbb{E} L(\boldsymbol{\theta})$ is linear in $\boldsymbol{\theta}$, it holds

$$\begin{aligned} L_G(\boldsymbol{\theta} + \mathbf{u}) - L_G(\boldsymbol{\theta}) - \langle \nabla L_G(\boldsymbol{\theta}), \mathbf{u} \rangle \\ = f(\boldsymbol{\theta} + \mathbf{u}) - f(\mathbf{u}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle. \end{aligned}$$

Therefore, it suffices to bound the ratio

$$\rho(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \frac{\int_{\mathcal{U}^c} \exp\{f(\boldsymbol{\theta} + \mathbf{u}) - f(\mathbf{u}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle\} d\mathbf{u}}{\int_{\mathcal{U}} \exp\{f(\boldsymbol{\theta} + \mathbf{u}) - f(\mathbf{u}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle\} d\mathbf{u}}$$

for the elliptic set $\mathcal{U} = \mathcal{U}(\boldsymbol{\theta}, \mathbf{r}_0) = \{\mathbf{u}: \|D(\boldsymbol{\theta})\mathbf{u}\| \leq \mathbf{r}_0\}$ uniformly in $\boldsymbol{\theta}$ from the set $\{\boldsymbol{\theta}: \|D_G(\boldsymbol{\theta} - \boldsymbol{\theta}_G^*)\| \leq \mathbf{r}_G\}$; see Theorem 2.

First we present some bounds for the denominator of $\rho(\boldsymbol{\theta})$. Local smoothness of $f(\boldsymbol{\theta}) = \mathbb{E} L_G(\boldsymbol{\theta})$ implies

$$\begin{aligned} & \int_{\mathcal{U}} \exp\{f(\boldsymbol{\theta} + \mathbf{u}) - f(\mathbf{u}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle\} d\mathbf{u} \\ & \approx \int_{\mathcal{U}} \exp\left(-\frac{\|D_G(\boldsymbol{\theta})\mathbf{u}\|^2}{2}\right) d\mathbf{u}, \end{aligned}$$

Moreover,

$$\frac{\det D_G(\boldsymbol{\theta})}{(2\pi)^{p/2}} \int_{\mathcal{U}} \exp\left(-\frac{\|D_G(\boldsymbol{\theta})\mathbf{u}\|^2}{2}\right) d\mathbf{u} = \mathbb{P}(\|D(\boldsymbol{\theta})D_G^{-1}(\boldsymbol{\theta})\boldsymbol{\gamma}\| \leq r_0)$$

for $\boldsymbol{\gamma} \sim \mathcal{N}(0, I_p)$. The choice $r_0 \geq \sqrt{p_G(\boldsymbol{\theta})} + \sqrt{2x}$ yields

$$\mathbb{P}(\|D(\boldsymbol{\theta})D_G^{-1}(\boldsymbol{\theta})\boldsymbol{\gamma}\| \leq r_0) \geq 1 - e^{-x}.$$

$f(\boldsymbol{\theta}) = \mathbb{E}L(\boldsymbol{\theta})$ is concave and $-\langle \nabla^2 f(\boldsymbol{\theta}) \mathbf{u}, \mathbf{u} \rangle = \|D(\boldsymbol{\theta}) \mathbf{u}\|^2$.

For any $\mathbf{u}$ with $\|D(\boldsymbol{\theta}) \mathbf{u}\| = r > r_0$

$$\begin{aligned} f(\boldsymbol{\theta} + \mathbf{u}) - f(\boldsymbol{\theta}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle - \|G\mathbf{u}\|^2/2 \\ \leq -C_0(\|D(\boldsymbol{\theta}) \mathbf{u}\| r_0 - r_0^2/2) - \|G\mathbf{u}\|^2/2 \\ = -C_0(\|D(\boldsymbol{\theta}) \mathbf{u}\| r_0 - r_0^2/2) - \|D_G(\boldsymbol{\theta}) \mathbf{u}\|^2/2 + \|D(\boldsymbol{\theta}) \mathbf{u}\|^2/2. \end{aligned}$$

with $C_0 \geq 1/2$ and $D_G^2(\boldsymbol{\theta}) = D^2(\boldsymbol{\theta}) + G^2$.

Now we can use the result about Gaussian integrals:

$$\begin{aligned} \frac{\det D_G}{(2\pi)^{p/2}} \int_{\|D\mathbf{u}\| \geq r_0} \exp\{- (\|D\mathbf{u}\| r_0 - r_0^2/2 - \|D_G\mathbf{u}\|^2 + \|D\mathbf{u}\|^2)/2\} d\mathbf{u} \\ \leq C e^{-(p_G(\boldsymbol{\theta}) + x)/2}. \end{aligned}$$

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- van der Vaart, A. W. , van Zanten, J. H. (2008)
- Leahu, H. (2011). Gaussian models
- Castillo, I. , Nickl, R. (2013, 2014). General results.
- Panov and Sp (2015). Semiparametric problems

Contraction results and local quadratic approximation of the log-likelihood. The Gaussian approximation in a weak sense.

Theorem

Suppose that It holds on $\Omega(\mathbf{x})$ with $\tilde{D}_G^2 = D_G^2(\tilde{\boldsymbol{\theta}}_G)$

$$\sup_{A \in \mathcal{B}_s(\mathbb{R}^p)} \left| \mathbb{P}(\boldsymbol{\vartheta}_G - \tilde{\boldsymbol{\theta}}_G \in A \mid \mathbf{Y}) - \mathbb{P}'(\tilde{D}_G^{-1} \boldsymbol{\gamma} \in A) \right| \leq \mathbf{C} \diamond(\mathbf{r}_0)$$

$$\sup_{A \in \mathcal{B}(\mathbb{R}^p)} \left| \mathbb{P}(\boldsymbol{\vartheta}_G - \tilde{\boldsymbol{\theta}}_G \in A \mid \mathbf{Y}) - \mathbb{P}'(\tilde{D}_G^{-1} \boldsymbol{\gamma} \in A) \right| \leq \mathbf{C} \delta_3(\mathbf{r}_0)$$

with

$$\delta_3(\mathbf{r}_0) \lesssim \frac{\mathbf{r}_0^3}{\sqrt{n}} \lesssim \frac{\mathbf{p}_G^{3/2}}{\sqrt{n}},$$

$$\diamond(\mathbf{r}_0) \lesssim \frac{\mathbf{r}_0^6}{n} \lesssim \frac{\mathbf{p}_G^3}{n}.$$

Fix any centrally symmetric set A . First we restrict the posterior probability to the set $\tilde{A}(\mathbf{r}_0) = \{\mathbf{u} : \|\tilde{D}\mathbf{u}\| \leq \mathbf{r}_0\}$. Then we apply the quadratic approximation of the log-likelihood function $L(\boldsymbol{\theta})$. Denote $A(\mathbf{r}_0) = A \cap \tilde{A}(\mathbf{r}_0)$. Obviously, $A(\mathbf{r}_0)$ is centrally symmetric as well. Further,

$$\begin{aligned} \mathbb{P}(\boldsymbol{\vartheta}_G - \tilde{\boldsymbol{\theta}}_G \in A \mid \mathbf{Y}) &= \frac{\int_A \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u})\} d\mathbf{u}}{\int_{\mathbb{R}^p} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u})\} d\mathbf{u}} \\ &\leq \frac{\int_{A(\mathbf{r}_0)} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u}) - L_G(\tilde{\boldsymbol{\theta}}_G) - \langle \nabla L_G(\tilde{\boldsymbol{\theta}}_G), \mathbf{u} \rangle\} d\mathbf{u}}{\int_{\tilde{A}(\mathbf{r}_0)} \exp\{L_G(\tilde{\boldsymbol{\theta}}_G + \mathbf{u}) - L_G(\tilde{\boldsymbol{\theta}}_G) - \langle \nabla L_G(\tilde{\boldsymbol{\theta}}_G), \mathbf{u} \rangle\} d\mathbf{u}} + \rho(\mathbf{r}_0). \end{aligned}$$

Fix $\boldsymbol{\theta} \in \mathcal{A}_G(\mathbf{r}_G)$. Then for $A \subset \mathcal{U}$ centrally symmetric

$$\begin{aligned} & \int_A \exp\{f(\boldsymbol{\theta} + \mathbf{u}) - f(\mathbf{u}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle\} d\mathbf{u} \\ & \geq (1 - \diamond(\mathbf{r}_0)) \int_A \exp\left(-\frac{\|D_G(\boldsymbol{\theta})\mathbf{u}\|^2}{2}\right) d\mathbf{u}, \\ & \int_A \exp\{f(\boldsymbol{\theta} + \mathbf{u}) - f(\mathbf{u}) - \langle \nabla f(\boldsymbol{\theta}), \mathbf{u} \rangle\} d\mathbf{u} \\ & \leq (1 + \diamond(\mathbf{r}_0)) \int_A \exp\left(-\frac{\|D_G(\boldsymbol{\theta})\mathbf{u}\|^2}{2}\right) d\mathbf{u}, \end{aligned}$$

where $\diamond(\mathbf{r}_0) = 4\delta_3^2 + 4\delta_4$.

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Consider the model

$$\mathbf{Y} = A(\mathbf{f}^*) + \sigma \boldsymbol{\varepsilon} \in \mathcal{Y}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(0, I) \quad (1)$$

with a known non-linear operator $A: \mathcal{X} \rightarrow \mathcal{Y}$ for Hilbert spaces $\mathcal{X}, \mathcal{Y}$.

We assume that A is injective and denote by $\mathfrak{A}$ its inverse:

$$\mathfrak{A} \stackrel{\text{def}}{=} A^{-1}: \mathcal{Y} \rightarrow \mathcal{X}.$$

A Gaussian log-likelihood in the model (1) w.r.t. $\mathbf{f}$ is of the form

$$L(\mathbf{f}) = -(2\sigma^2)^{-1} \|\mathbf{Y} - A(\mathbf{f})\|^2.$$

A Gaussian prior $\mathbf{f} \sim \mathcal{N}(\mathbf{f}_0, G^{-2})$ yields the penalized log-likelihood

$$\mathcal{L}_G(\mathbf{f}) = -(2\sigma^2)^{-1} \|\mathbf{Y} - A(\mathbf{f})\|^2 - \frac{1}{2} \|G(\mathbf{f} - \mathbf{f}_0)\|^2.$$

However, it does not satisfy the crucial conditions $(\mathcal{L})$ and (E) .

One can use another parametrization by $\mathbf{g} = A(\mathbf{f}) \in \mathcal{Y}$ where $\mathbf{g}$ is “smooth”. This yields the classical log-likelihood

$$L(\mathbf{g}) = -\frac{1}{2\sigma^2} \|\mathbf{Y} - \mathbf{g}\|^2.$$

Let now $\mathbf{f} \sim \mathcal{N}(\mathbf{f}_0, G^{-2})$. It leads to a non-Gaussian prior $\mathfrak{A}(\mathbf{g})$ on $\mathcal{Y}$. The penalized log-likelihood $\mathcal{L}_G(\mathbf{g})$ reads

$$\mathcal{L}_G(\mathbf{g}) = -\frac{1}{2\sigma^2} \|\mathbf{Y} - \mathbf{g}\|^2 - \frac{1}{2} \|G \{\mathfrak{A}(\mathbf{g}) - \mathbf{f}_0\}\|^2 + \mathbf{c}.$$

Further, it holds for the expected log-likelihood

$$\mathbb{E} \mathcal{L}_G(\boldsymbol{\eta}) = -\frac{1}{2\sigma^2} \|A(\mathbf{f}^*) - \mathbf{g}\|^2 - \frac{1}{2} \|G \{\mathfrak{A}(\mathbf{g}) - \mathbf{f}_0\}\|^2 + \mathbf{c}$$

Problem: $\mathfrak{A}$ unbounded and non-smooth.

Represent $\mathbf{Y} = A(\mathbf{f}) + \sigma\boldsymbol{\varepsilon}$ by two identities $\mathbf{Y} = \mathbf{g} + \sigma\boldsymbol{\varepsilon}$ and $\mathbf{g} = A(\mathbf{f})$. Then the fidelity terms can be relaxed to

$$\sigma^{-2} \|\mathbf{Y} - \mathbf{g}\|^2 + \lambda \|\mathbf{g} - A(\mathbf{f})\|^2.$$

Bayesian modeling assumes regular priors on $\mathbf{g}$ and $\mathbf{f}$. In particular, one can use Gaussian priors $\mathbf{f} \sim \mathcal{N}(\mathbf{f}_0, G^{-2})$ and $\mathbf{g} \sim \mathcal{N}(\mathbf{g}_0, \Gamma^{-2})$ yielding the posterior

$$\begin{aligned} \mathbf{f}, \mathbf{g} \mid \mathbf{Y} &\propto \exp \mathcal{L}_G(\mathbf{f}, \mathbf{g}) \\ \mathcal{L}_G(\mathbf{f}, \mathbf{g}) &= -\frac{1}{2\sigma^2} \|\mathbf{Y} - \mathbf{g}\|^2 - \frac{\lambda}{2} \|\mathbf{g} - A(\mathbf{f})\|^2 \\ &\quad - \frac{1}{2} \langle \mathbf{f} - \mathbf{f}_0 \rangle_G - \frac{1}{2} \langle \mathbf{g} - \mathbf{g}_0 \rangle_\Gamma. \end{aligned}$$

The gradient and Hessian of $\mathcal{L}_G(\mathbf{f}, \mathbf{g})$ read as follow:

$$\frac{d}{d\mathbf{f}} \mathcal{L}_G(\mathbf{f}, \mathbf{g}) = -\lambda \{A(\mathbf{f}) - \mathbf{g}\}^\top \nabla A(\mathbf{f}) - G^2(\mathbf{f} - \mathbf{f}_0)$$

$$\frac{d}{d\mathbf{g}} \mathcal{L}_G(\mathbf{f}, \mathbf{g}) = \sigma^{-2}(\mathbf{Y} - \mathbf{g}) + \lambda \{A(\mathbf{f}) - \mathbf{g}\} - \Gamma^2(\mathbf{g} - \mathbf{g}_0)$$

and

$$\begin{aligned} \mathbb{F}(\mathbf{f}, \mathbf{g}) &\stackrel{\text{def}}{=} -\nabla^2 \mathbb{E} \mathcal{L}_G(\mathbf{f}, \mathbf{g}) \\ &= \begin{pmatrix} G^2 + \lambda (\nabla^\top \nabla + \boldsymbol{\delta}^\top \nabla^2) A(\mathbf{f}) & \lambda \nabla A(\mathbf{f}) \\ \lambda \{\nabla A(\mathbf{f})\}^\top & \Gamma^2 + (\sigma^{-2} + \lambda) I \end{pmatrix} \end{aligned}$$

with the elasticity vector $\boldsymbol{\delta} = A(\mathbf{f}) - \mathbf{g}$. For convexity of $-\mathbb{E} \mathcal{L}_G(\mathbf{f}, \mathbf{g})$ it suffices to check that $\nabla^2 \mathbb{E} \mathcal{L}_G(\mathbf{f}, \mathbf{g}) < 0$.

In a special case when A is linear and $\nabla A(\mathbf{f}) = A$, it holds $\nabla^2 A = 0$ and the matrix $\mathbb{F}(\mathbf{f}, \mathbf{g})$ does not depend on $(\mathbf{f}, \mathbf{g})$:

$$\mathbb{F} = -\nabla^2 \mathbb{E} \mathcal{L}_G(\mathbf{f}, \mathbf{g}) = \begin{pmatrix} G^2 + \lambda A^\top A & \lambda A \\ \lambda A^\top & \Gamma^2 + (\sigma^{-2} + \lambda)I \end{pmatrix}.$$

With $G^2 > 0$ and $\Gamma^2 > 0$, this matrix is also positive semidefinite.

The $\mathbf{f}\mathbf{f}$ -block of the matrix $\mathbb{F}^{-1}$ reads

$$\begin{aligned} (\mathbb{F}^{-1})_{\mathbf{f}\mathbf{f}} &= (\mathbb{F}_{\mathbf{f}\mathbf{f}} - \mathbb{F}_{\mathbf{f}\mathbf{g}} \mathbb{F}_{\mathbf{g}\mathbf{g}}^{-1} \mathbb{F}_{\mathbf{g}\mathbf{f}})^{-1} \\ &= (G^2 + \lambda A^\top A)^{-1} - \lambda^2 A^\top \{\Gamma^2 + (\sigma^{-2} + \lambda)I\}^{-1} A. \end{aligned}$$

One can see that each of regularizations by G^2 and Γ^2 improves the conditioning number of $\mathbb{F}_{\mathbf{f}\mathbf{f}} - \mathbb{F}_{\mathbf{f}\mathbf{g}} \mathbb{F}_{\mathbf{g}\mathbf{g}}^{-1} \mathbb{F}_{\mathbf{g}\mathbf{f}}$. Moreover, one can use $\lambda = \sigma^{-2}$ yielding $(\mathbb{F}^{-1})_{\mathbf{f}\mathbf{f}} \asymp \mathbb{F}_{\mathbf{f}\mathbf{f}}^{-1} = \{G^2 + \sigma^{-2} A^\top A\}^{-1}$.

In the case of a non-linear operator A

$$\begin{aligned}\mathbb{F}(\mathbf{f}, \mathbf{g}) &\stackrel{\text{def}}{=} -\nabla^2 \mathbb{E} \mathcal{L}_G(\mathbf{f}, \mathbf{g}) \\ &= \begin{pmatrix} G^2 + \lambda (\nabla^\top \nabla + \boldsymbol{\delta}^\top \nabla^2) A(\mathbf{f}) & \lambda \nabla A(\mathbf{f}) \\ \lambda \{\nabla A(\mathbf{f})\}^\top & \Gamma^2 + (\sigma^{-2} + \lambda) I \end{pmatrix}\end{aligned}$$

with the elasticity vector $\boldsymbol{\delta} = A(\mathbf{f}) - \mathbf{g}$.

The only term in the matrix $\mathbb{F}(\mathbf{f}, \mathbf{g})$ involving the second derivative of $A(\cdot)$ appears in the $\mathbf{f}\mathbf{f}$ -block with the multiplicative elasticity factor $\boldsymbol{\delta} = A(\mathbf{f}) - \mathbf{g}$.

If the structural equation $A(\mathbf{f}) = \mathbf{g}$ is nearly fulfilled, then this factor vanishes and the impact of this nonlinearity disappears.

The partial penalized MLE in $\mathbf{g}$ given $\mathbf{f}$ can be computed explicitly. The equation $\frac{d}{d\mathbf{g}}\mathcal{L}_G(\mathbf{f}, \mathbf{g}) = 0$ yields

$$\tilde{\mathbf{g}}(\mathbf{f}) = \{(\sigma^{-2} + \lambda)I + \Gamma^2\}^{-1} \{\sigma^{-2}\mathbf{Y} + \lambda A(\mathbf{f}) + \Gamma^2 \mathbf{g}_0\}.$$

With $\boldsymbol{\eta}$ fixed, optimization w.r.t. $\mathbf{f}$ yields the equation

$$\lambda \{A(\mathbf{f}) - \mathbf{g}\}^\top \nabla A(\mathbf{f}) = -G^2(\mathbf{f} - \mathbf{f}_0).$$

With a guess $\mathbf{f}^\circ$ and $\boldsymbol{\delta} = A(\mathbf{f}^\circ) - \mathbf{g}$, one gets

$A(\mathbf{f}) \approx A(\mathbf{f}^\circ) + \nabla A(\mathbf{f}^\circ)(\mathbf{f} - \mathbf{f}^\circ)$ and

$\nabla A(\mathbf{f}) \approx \nabla A(\mathbf{f}^\circ) + \nabla^2 A(\mathbf{f}^\circ)(\mathbf{f} - \mathbf{f}^\circ)$. This yields an update

$$\begin{aligned} \mathbf{f} - \mathbf{f}^\circ &= \{G^2 + \lambda(\nabla^\top \nabla + \boldsymbol{\delta}^\top \nabla^2)A(\mathbf{f}^\circ)\}^{-1} \\ &\quad \times [G^2(\mathbf{f}^\circ - \mathbf{f}_0) + \lambda \boldsymbol{\delta}^\top \nabla A(\mathbf{f}^\circ)] \end{aligned}$$

Now we present a result about large deviation bound for the penalized MLE. Let

$$\tilde{\mathbf{v}}_G = (\tilde{\mathbf{f}}_G, \tilde{\mathbf{g}}_G) \stackrel{\text{def}}{=} \operatorname{argmax}_{\mathbf{v} \in \mathcal{Y}^o} \mathcal{L}_G(\mathbf{v}).$$

Under condition (ED_0) , for any $\mathbf{x} > 0$ there exists a random set $\Omega(\mathbf{x})$ with $\mathbb{P}(\Omega(\mathbf{x})) \geq 1 - Ce^{-\mathbf{x}}$ such that $\nabla_{\mathbf{g}} \zeta(\mathbf{g})$ satisfies

$$\|D_G^{-1} \nabla_{\mathbf{g}} \zeta\| \leq z(B_{V|G}, \mathbf{x}) \text{ on } \Omega(\mathbf{x}),$$

where $B_{V|G} = D_G^{-1} V^2 D_G^{-1}$ and for any matrix B

$$z(B, x) = \sqrt{\operatorname{tr} B} + \sqrt{2\lambda_{\max}(B)x}.$$

Theorem

Let $\|D_G^{-1}\nabla_g\zeta\| \leq z(B_{V|G}, \mathbf{x})$ hold on a random set $\Omega(\mathbf{x})$ with $\mathbb{P}(\Omega(\mathbf{x})) \geq 1 - e^{-x}$ and

$$r_G \geq 2z(B_{V|G}, \mathbf{x}).$$

Then on $\Omega(\mathbf{x})$

$$\|\mathcal{D}_G(\tilde{\mathbf{v}}_G - \mathbf{v}_G^*)\| \leq r_G.$$

This also implies

$$\|D_G(\tilde{\mathbf{f}}_G - \mathbf{f}_G^*)\| \leq r_G.$$

Theorem

Let

$$C_0 r_0 \geq 2\sqrt{p_G(\mathbf{v})} + \sqrt{x}, \quad \mathbf{v} \in \mathcal{Y}_0.$$

Then, on the random set $\Omega(\mathbf{x})$ from Theorem 5, the quantity

$$\rho(\mathbf{r}_0) \stackrel{\text{def}}{=} \frac{\int_{\|\tilde{\mathcal{D}}\mathbf{u}\| \geq r_0} \exp\{L_G(\tilde{\mathbf{v}}_G + \mathbf{u})\} d\mathbf{u}}{\int_{\|\tilde{\mathcal{D}}\mathbf{u}\| \leq r_0} \exp\{L_G(\tilde{\mathbf{v}}_G + \mathbf{u})\} d\mathbf{u}}$$

fulfills

$$\rho(\mathbf{r}_0) \leq 2 \exp\{-(\tilde{p}_G + x)/2\},$$

where $\tilde{p}_G = p_G(\tilde{\mathbf{v}}_G)$.

Corollary

It holds on $\Omega(\mathbf{x})$

$$\sup_{A \in \mathcal{B}_s(\mathcal{Y}^d)} \left| \mathbb{P}(\mathbf{v}_G - \tilde{\mathbf{v}}_G \in A \mid \mathbf{Y}) - \mathbb{P}'(\tilde{\mathcal{D}}_G^{-1} \boldsymbol{\gamma} \in A) \right| \lesssim \diamond(\mathbf{r}_0)$$
$$\sup_{A \in \mathcal{B}(\mathcal{Y}^d)} \left| \mathbb{P}(\mathbf{v}_G - \tilde{\mathbf{v}}_G \in A \mid \mathbf{Y}) - \mathbb{P}'(\tilde{\mathcal{D}}_G^{-1} \boldsymbol{\gamma} \in A) \right| \lesssim \delta_3(\mathbf{r}_0).$$

Finally we state the result about the marginal posterior $\mathbf{f}_G \mid \mathbf{Y}$.

Corollary

It holds on $\Omega(\mathbf{x})$

$$\sup_{A \in \mathcal{B}_s(\mathcal{X}^d)} \left| \mathbb{P}(\mathbf{f}_G - \tilde{\mathbf{f}}_G \in A \mid \mathbf{Y}) - \mathbb{P}'(\tilde{D}_G^{-1} \boldsymbol{\gamma} \in A) \right| \lesssim \diamond(\mathbf{r}_0)$$
$$\sup_{A \in \mathcal{B}(\mathcal{X}^d)} \left| \mathbb{P}(\mathbf{f}_G - \tilde{\mathbf{f}}_G \in A \mid \mathbf{Y}) - \mathbb{P}'(\tilde{D}_G^{-1} \boldsymbol{\gamma} \in A) \right| \lesssim \delta_3(\mathbf{r}_0).$$