TUBAF

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Sensitivity of uncertainty propagation, risk, and Bayesian inversion

Joint work with Oliver Ernst and Alois Pichler (TU Chemnitz)

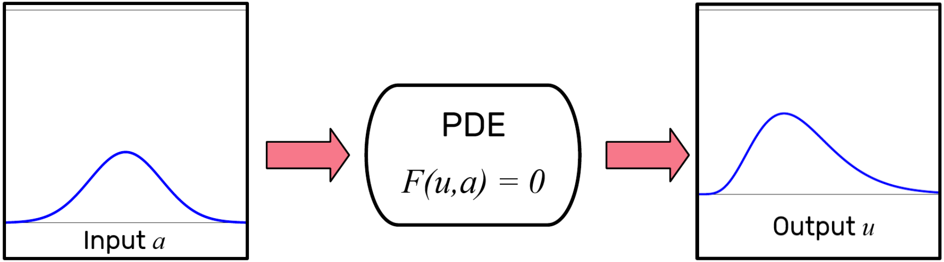
Björn Sprungk

Workshop “Uncertainty Quantification for High-Dimensional Problems”, CWI Amsterdam

November 13th, 2024

Uncertainty Propagation

UQ scheme



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Can we control the effect of perturbations of μ on output distribution ν?

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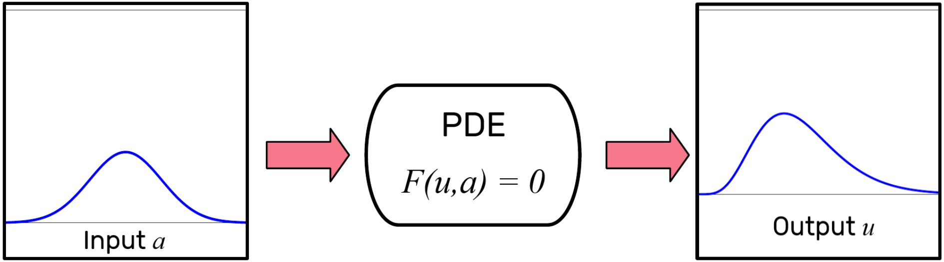

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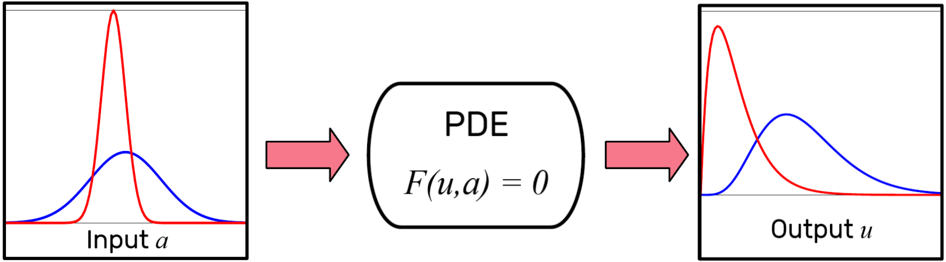

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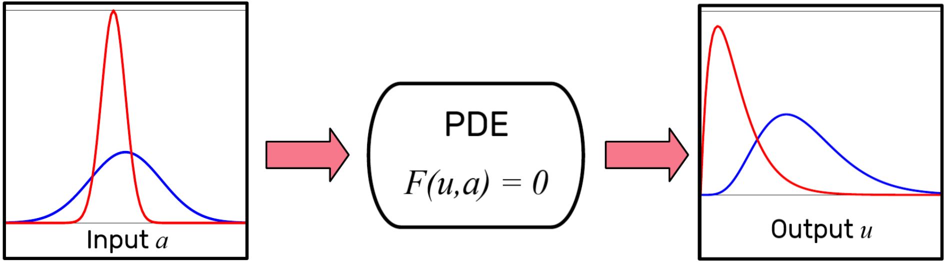

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Setting

- Consider general PDE with solution $u \in \mathscr{U}$ and uncertain coefficient(s) $a \in \mathscr{A}$ given by

$$\mathscr{F}(u, a) = 0$$

  with associated solution operator $S \colon \mathscr{A} \to \mathscr{U}$ mapping coefficient a to unique solution u

- **Running example**: Elliptic diffusion equation on compact $D \subseteq \mathbb{R}^2$,

$$-\nabla \cdot (\mathrm{e}^{a} \nabla u) = f, \qquad u\big|_{\partial D} \equiv 0$$

  with $\mathscr{U} = H_0^1(D)$ and $\mathscr{A} = L^\infty(D)$ (weak form)

- **UQ approach:**
  1. Describe uncertainty about a by probability measure μ on $\mathscr{A}$
  2. Compute pushforward distribution $S_*\mu$ on $\mathscr{U}$ of random solution $u = S(a)$, $a \sim \mu$

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Gaussian random fields as coefficients

- Often we assume $a \sim \mathrm{N}(m, c)$ with mean and covariance function m and c

$$\mathrm{E}\left[a(x)\right] = m(x), \qquad \mathrm{Cov}[a(x), a(y)] = c(x, y), \qquad a(x) \sim \mathrm{N}\left(m(x), c(x, x)\right)$$

- Common parametrized class: Matérn covariance functions

$$c_{\sigma^2,\rho,k+\frac{1}{2}}(x, y) := \sigma^2 \, \mathrm{e}^{-\frac{\sqrt{2k+1}}{\rho}|x-y|} \, P_k\left(\frac{\sqrt{2k+1}}{\rho}|x - y|\right)$$

with variance $\sigma^2 > 0$, correlation length $\rho > 0$, smoothness $k + \frac{1}{2}$, $k \in \mathbb{N}_0$

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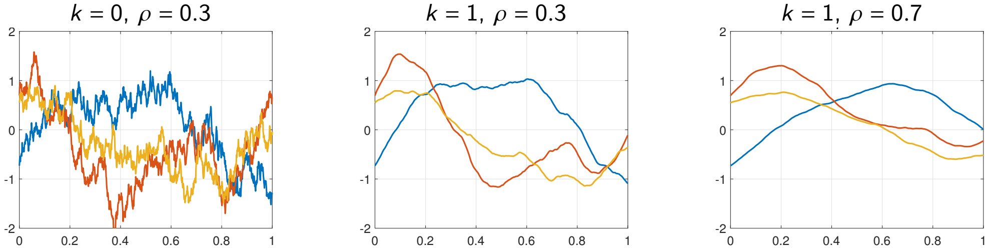

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- **In practice:** Use estimates $\widehat{\sigma}^2$, $\widehat{k}$, $\widehat{\rho}$ given data $a(x_j), j = 1, \ldots, n$

Motivational Question

How does estimation error, e.g., for σ^2, affect the output of the UQ analysis?

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Smoothness of forward map

- Often forward map S is (locally) Lipschitz: with monotonically increasing $\mathrm{Lip}_S : \mathbb{R}_+ \to \mathbb{R}_+$

$$\|S(a) - S(\widehat{a})\|_{\mathscr{U}} \le \mathrm{Lip}_S(r) \; \|a - \widehat{a}\|_{\mathscr{A}} \qquad \forall \|a\|_{\mathscr{A}}, \|\widehat{a}\|_{\mathscr{A}} \le r$$

- **Running example:** For elliptic problem $-\nabla \cdot (\mathrm{e}^a \nabla u) = f$ we have if $\|a\|_{L^\infty(D)}, \|\widehat{a}\|_{L^\infty(D)} \le r$

$$\|u - \widehat{u}\|_{H_0^1(D)} = \|S(a) - S(\widehat{a})\|_{H_0^1(D)} \le c_f \, \mathrm{e}^{3r} \; \|a - \widehat{a}\|_{L^\infty(D)}$$

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Suitable Metric

- Common choice: total variation distance

$$d_{\mathrm{TV}}(\mu, \widehat{\mu}) = \sup_{A \subseteq \mathscr{A}} |\mu(A) - \widehat{\mu}(A)| = \frac{1}{2} \sup_{f \colon \|f\|_{L^\infty} \le 1} \left| \mathrm{E}_{X \sim \mu}[f(X)] - \mathrm{E}_{X \sim \widehat{\mu}}[f(X)] \right|$$

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$$d_{\mathrm{TV}}(S_* \mu, S_* \widehat{\mu}) \le d_{\mathrm{TV}}(\mu, \widehat{\mu}), \qquad \text{for any measurable } S \colon \mathscr{A} \to \mathscr{U}$$

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Wasserstein distance

- Instead, we consider the p-Wasserstein distance, $p \geq 1$,

$$\mathrm{W}_p(\mu, \widehat{\mu}) := \inf_{X \sim \mu,\ \widehat{X} \sim \widehat{\mu}} \mathrm{E}\left[\|X - \widehat{X}\|^p\right]^{1/p}$$

- We have $\mathrm{W}_p(\mu, \widehat{\mu}) \leq \mathrm{W}_{p'}(\mu, \widehat{\mu})$ for $p \leq p'$ and

$$\mathrm{W}_1(\mu, \widehat{\mu}) = \sup_{f:\ \mathrm{Lip}_f \leq 1} \left|\mathrm{E}_{X \sim \mu}\left[f(X)\right] - \mathrm{E}_{X \sim \widehat{\mu}}\left[f(X)\right]\right|$$

- Also reasonable for measures which are singular w. r. t. each other, e. g., W_2-distance of Gaussian random field measures explicitly known [Gelbrich, 1990][1]

[1] M. Gelbrich. On a Formula for the L2 Wasserstein Metric between Measures on Euclidean and Hilbert Spaces. *Mathematische Nachrichten* **147(1)**:185-203, 1990.

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Theorem (Wasserstein sensitivity)

Let $S\colon \mathscr{A} \to \mathscr{U}$ be globally Lipschitz,

$$\|S(a) - S(\widehat{a})\|_{\mathscr{U}} \le \mathrm{Lip}_S \, \|a - \widehat{a}\|_{\mathscr{A}} \qquad \forall \|a\|_{\mathscr{A}}, \|\widehat{a}\|_{\mathscr{A}} < \infty.$$

Then for any $\mu, \widehat{\mu}$ we have

$$\mathrm{W}_p\left(S_*\mu, S_*\widehat{\mu}\right) \le \mathrm{Lip}_S \mathrm{W}_p\left(\mu, \widehat{\mu}\right), \qquad p \ge 1.$$

If S is not globally Lipschitz, then $\mu \mapsto S_*\mu$ as well: for $\mu = \mathrm{N}(0,1)$, $\mu_n = \mathrm{N}(n,1)$, $S(x) := e^x$, $x \in \mathbb{R}$,

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Then for any $\mu, \widehat{\mu}$ with

$$\mathrm{E}_{\mu}\left[\mathrm{Lip}_S^{2p}(\|a\|_{\mathscr{A}})\right],\ \mathrm{E}_{\widehat{\mu}}\left[\mathrm{Lip}_S^{2p}(\|a\|_{\mathscr{A}})\right] \le C < \infty$$

we have

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Special case: Gaussian random fields

- Consider **subclass $\mathscr{G}$ of Gaussian measures on** $C(D)$ **with Matérn covariance** $c_{\sigma^2,\rho,k+\frac{1}{2}}$

$$\mathscr{G} = \left\{ \mathrm{N}\left(m, c_{\sigma^2,\rho,k+\frac{1}{2}}\right) : \|m\|_{C(D)} \leq M, \quad \sigma \leq \sigma_{\max}, \quad \rho \geq \rho_{\min}, \quad k \in \{0, \ldots, k_{\max}\} \right\}$$

- Fernique's theorem + Dudley's entropy bound yield $\sup_{\mu \in \mathscr{G}} \mathrm{E}_{a\sim\mu}\left[\exp\left(\beta \|a\|_{C(D)}\right)\right] < \infty, \beta > 0$

Theorem

If $S\colon C(D) \to \mathscr{U}$ is locally Lipschitz with $\mathrm{Lip}_S(r) \in \mathscr{O}(e^{\beta r})$ for a $\beta > 0$, then, there exists a constant $C = C(\mathscr{G}) < \infty$ such that

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Related work

- [Amir Sagev, 2020][2]: Upper and lower bounds for

$$\mathrm{W}_p\left(S_*\mu, \widetilde{S}_*\mu\right)$$

  for approximations $\widetilde{S}$ of forward map $S\colon \mathscr{A} \to \mathscr{U}$, e.g., numerical approximations

- [Owhadi et al., 2013][3]: Robust UQ in terms of upper and lower bounds on failure probabilities

$$\mathrm{P}_{a\sim\mu}(q(u) > \mathrm{tol})$$

  by varying (μ, q) or $(\mu, q \circ S)$ within an admissible set of input distributions and forward maps

[2] A. Sagiv. The Wasserstein distances between pushed-forward measures with applications to uncertainty quantification. *Commun. Math. Sci.* **18(3)**:707–724, 2020.

[3] H. Owhadi, C. Sovel, T. Sullivan, M. McKerns, M. Ortiz. Optimal Uncertainty Quantification. *SIAM Review* **55(2)**:271–345, 2013.

Risk

Risk Functionals

- Consider now scalar quantity of interest $q\colon \mathscr{U} \to \mathbb{R}$ of solution u of (random) PDE
- Risk functionals R assign real numbers $\mathrm{R}(X) \in \mathbb{R}$ to (real-valued) random variables X which quantify the risk associated with their random outcomes:

Expectation:	$\mathrm{R}(X) = \mathrm{E}[X]$	
Value-at-Risk (VaR):	$\mathrm{R}(X) := F_X^{-1}(1-\alpha),$	$\alpha \in (0,1)$
Average Value-at-Risk (AVaR):	$\mathrm{R}(X) = \dfrac{1}{\alpha}\displaystyle\int_{1-\alpha}^{1} F_X^{-1}(t)\mathrm{d}t,$	$\alpha \in (0,1)$
Spectral risk functional:	$\mathrm{R}(X) = \displaystyle\int_0^1 w(t)\, F_X^{-1}(t)\mathrm{d}t,$	$w \in L^1(\mathbb{R}_+)$

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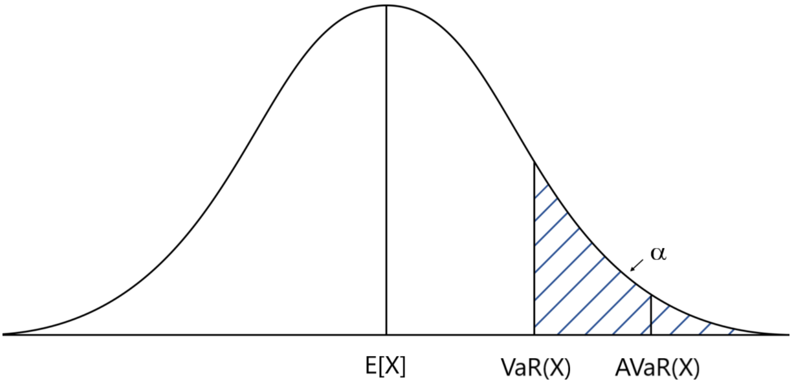

Question

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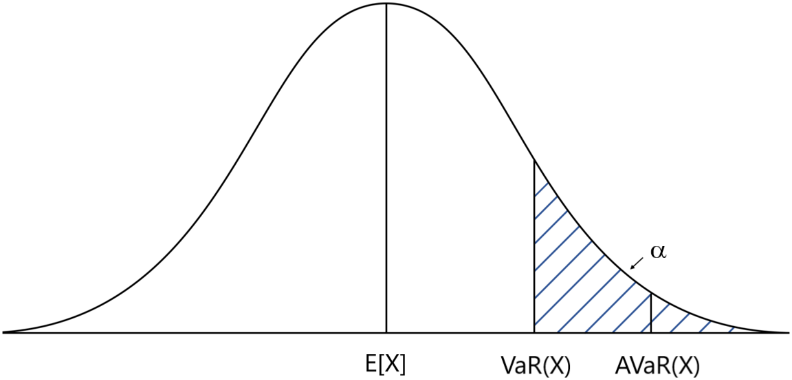

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Sensitivity of risk

For spectral risk functionals and larger class of coherent risk functionals [Artzner et al., 1997] we have dual representation

$$\mathrm{R}(X) = \sup_{Z \in \mathscr{Z}} \mathrm{E}\,[Z\, X]\,, \qquad \mathscr{Z} \subseteq \{Z \colon Z \geq 0 \text{ a. s. and } \mathrm{E}\,[Z] = 1\},$$

i.e., Z basically represent probability density functions

Theorem

For Hölder-continuous quantity $q \colon \mathscr{U} \to \mathbb{R}$, i.e., $|q(u) - q(\widehat{u})| \leq C_q \|u - \widehat{u}\|_{\mathscr{U}}^{\beta}$, $\beta > 0$, we have for any coherent risk functional R that

$$|\mathrm{R}(q(u)) - \mathrm{R}(q(\widehat{u}))| \leq C_{\mathrm{R},p,q}\, \mathrm{W}_p\,(\nu, \widehat{\nu})^{\beta}, \qquad p \geq 1$$

where $u \sim \nu$ and $\widehat{u} \sim \widehat{\nu}$.

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For Hölder-continuous quantity $q \colon \mathscr{U} \to \mathbb{R}$, i.e., $|q(u) - q(\widehat{u})| \leq C_q \|u - \widehat{u}\|_{\mathscr{U}}^{\beta}$, $\beta > 0$, we have for any coherent risk functional R that

$$|\mathrm{R}(q(u)) - \mathrm{R}(q(\widehat{u}))| \leq C_{\mathrm{R},p,q}\ \mathrm{W}_p\,(\nu, \widehat{\nu})^{\beta}, \qquad p \geq 1$$

where $u \sim \nu$ and $\widehat{u} \sim \widehat{\nu}$.

Corollary

For Hölder-continuous $q\colon \mathscr{U} \to \mathbb{R}$ and locally Lipschitz $S\colon \mathscr{A} \to \mathscr{U}$ we have for any spectral risk measures R and suitable measures $\mu, \widehat{\mu}$ on $\mathscr{A}$

$$|\mathrm{R}(q(u)) - \mathrm{R}(q(\widehat{u}))| \leq C_{q,w,p}\, \mathrm{W}_{2p}\,(\mu, \widehat{\mu})^{\beta}\,, \qquad p \geq 1,$$

where $u = S(a)$, $a \sim \mu$, and $\widehat{u} = S(\widehat{a})$, $\widehat{a} \sim \widehat{\mu}$.

Example: For elliptic problem $-\nabla \cdot (e^{a} \nabla u) = f$ with lognormal diffusion coefficients we have for $a \sim \mathrm{N}(m, c_{\sigma^2,\rho,k+\frac{1}{2}})$, $\widehat{a} \sim \mathrm{N}(m, c_{\widehat{\sigma}^2,\rho,k+\frac{1}{2}})$

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for Hölder-continuous $q\colon H_0^1(D) \to \mathbb{R}$

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Bayesian Inference

Bayesian approach to inverse problem

$$y = G(a) + \varepsilon, \qquad G: \mathscr{A} \to \mathbb{R}^k, \qquad \varepsilon \sim \mathrm{N}(0, \Sigma),$$

- Condition prior measure $a \sim \mu$ given data $y = G(a) + \varepsilon$ yields posterior measure

Bayes' rule

$$\mu_\Phi(\mathrm{d}a) \;\propto\; \mathrm{e}^{-\Phi(a)}\,\mu(\mathrm{d}a), \qquad \Phi(a) := \frac{1}{2}\|y - G(a)\|^2_{\Sigma^{-1}}.$$

- BIP well-posed, i.e., local Lipschitz dependence of μ_Φ on data $y \in \mathbb{R}^k$ [Stuart, 2010], [Hosseini, 2017], [Sullivan, 2017], [Latz, 2020],...

- **Question:** How sensitively depends posterior μ_Φ on (subjective) choice of prior μ ?

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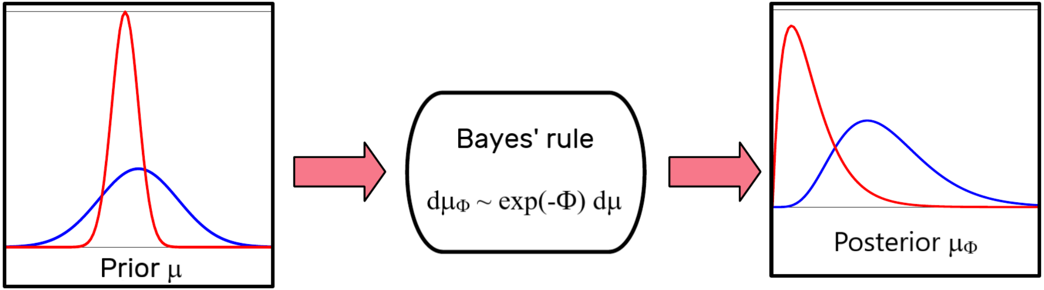
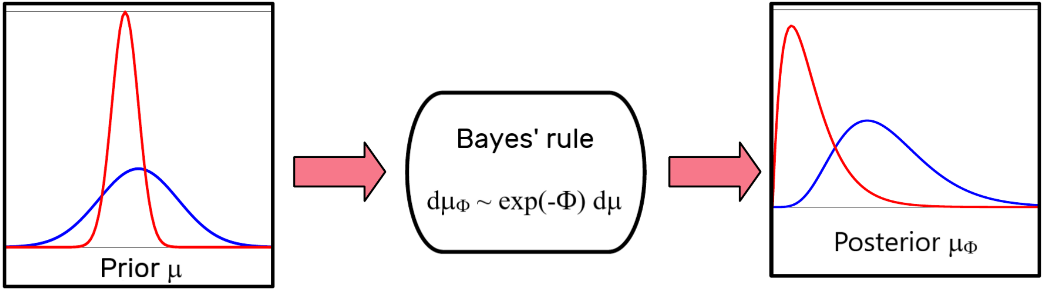


Theorem (informal)

For d being TV, Hellinger, or 1-Wasserstein distance or KL divergence we have under suitable assumptions a locally Lipschitz continuity:

$$d(\mu_\Phi, \widehat{\mu}_\Phi) \;\le\; C_\Phi(r)\; d(\mu, \widehat{\mu}), \qquad \text{if} \;\; d(\mu, \widehat{\mu}) \le r$$

But: $C_\Phi(r) \longrightarrow \infty$ as data y more informative, e.g., noise $\varepsilon \longrightarrow 0$



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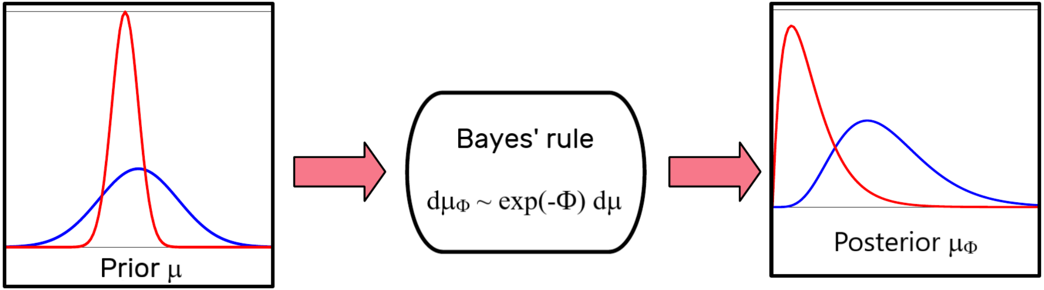

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- For the TV-distance, we have

$$d_{\mathrm{TV}}(\mu_\Phi, \widehat{\mu}_\Phi) \le \frac{2}{Z}\, d_{\mathrm{TV}}(\mu, \widehat{\mu}), \qquad Z := \int \mathrm{e}^{-\Phi} \mathrm{d}\mu$$

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Related work

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$$\Gamma_\epsilon(\mu) := \{(1-\epsilon)\mu + \epsilon\tilde{\mu} : \ \tilde{\mu} \in \mathscr{P}\}, \qquad \epsilon > 0$$

- [Diaconis & Freedman, 1986]: Fréchet derivative $\partial T_\Phi(\mu)$ of $T_\Phi(\mu) := \mu_\Phi$ w.r.t. TV topology

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- [Gustafson & Wasserman, 1995]: Sensitivity measure based on Gâteaux derivative w.r.t perturbations based with explicit growth for increasing number of i.i.d. data

- Bayesian brittleness [Owhadi et al., 2015]: Span of posterior expectations for $f : \mathscr{A} \to \mathbb{R}$ for all priors μ which satisfy finitely many generalized moment conditions coincides with range(f)

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