Robust estimation via Minimum Distance Estimation

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Statistical Estimation and Deep Learning in UQ for PDEs Vienna, May 2022

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- Complex models

3 A Bayesian(?) point of view

- 1st approach : "generalized posteriors"
- 2nd approach : ABC

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The Maximum Likelihood Estimator (MLE)

Let X_1, \ldots, X_n be i.i.d in \mathcal{X} from a probability distribution P_0 .

Statistical inference :

- propose a model $(P_{\theta}, \theta \in \Theta)$, assume $P_0 = P_{\theta_0}$.
- compute $\hat{\theta}_n = \hat{\theta}_n(X_1, \dots, X_n)$.

Letting p_{θ} denote the density of P_{θ} , then

$$\hat{\theta}_n^{MLE} = rgmax_{\theta\in\Theta} L_n(\theta)$$
, where $L_n(\theta) = \prod_{i=1}^n p_{\theta}(X_i)$.

Example : $P_{(m,\sigma)} = \mathcal{N}(m,\sigma^2)$ then

$$\hat{m} = \frac{1}{n} \sum_{i=1}^{n} X_i \text{ and } \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \hat{m})^2.$$

Some problems with the likelihood Minimum Distance Estimation (MDE)

MLE not unique / not consistent

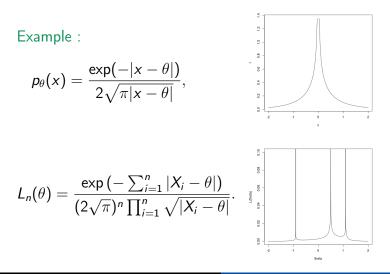
Example :

$$p_{ heta}(x) = rac{\exp(-|x- heta|)}{2\sqrt{\pi|x- heta|}},$$



Some problems with the likelihood Minimum Distance Estimation (MDE)

MLE not unique / not consistent



Some problems with the likelihood Minimum Distance Estimation (MDE)

MLE fails in the presence of outliers

What is an outlier?

Huber proposed the contamination model : with probability ε , X_i is not drawn from P_{θ_0} but from Q that can be anything :

$$P_0 = (1 - \varepsilon) P_{\theta_0} + \varepsilon Q.$$

Example : $P_{\theta} = Unif[0, \theta]$, then

$$L_n(\theta) = \frac{1}{\theta^n} \prod_{i=1}^n \mathbb{1}_{\{0 \le X_i \le \theta\}} \Rightarrow \hat{\theta} = \max_{1 \le i \le n} X_i.$$

In the case of the following contamination, the MLE is extremely far from the truth :

$$P_0 = (1 - \varepsilon) \mathcal{U}$$
nif $[0, 1] + \varepsilon \mathcal{N}(10^{10}, 1) \dots$

Some problems with the likelihood Minimum Distance Estimation (MDE)

Minimum Distance Estimation

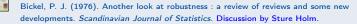
Minimum Distance Estimation (MDE)

Let $d(\cdot, \cdot)$ be a metric on probability distributions.

$$\hat{ heta}_d := rgmin_{ heta \in \Theta} d\left(P_ heta, \hat{P}_n
ight) \, ext{ where } \hat{P}_n := rac{1}{n} \sum_{i=1}^n \delta_{X_i}.$$

Wolfowitz, J. (1957). The minimum distance method. The Annals of Mathematical Statistics.

Idea : MDE with an adequate d leads to robust estimation.



Parr, W. C. & Schucany, W. R. (1980). Minimum distance and robust estimation. JASA.

Yatracos, Y. G. (1985). Rates of convergence of minimum distance estimators and Kolmogorov's entropy. *Annals of Statistics.*

Some problems with the likelihood Minimum Distance Estimation (MDE)

Integral Probability Semimetrics

Integral Probability Semimetrics (IPS)

Let ${\mathcal F}$ be a set of real-valued, measurable functions and put

$$d_{\mathcal{F}}(P,Q) = \sup_{f\in\mathcal{F}} \left| \mathbb{E}_{X\sim P}[f(X)] - \mathbb{E}_{X\sim Q}[f(X)] \right|.$$

Müller, A. (1997). Integral probability metrics and their generating classes of functions. *Applied Probability*.

- assumptions required in order to ensure that $d_{\mathcal{F}}(P, Q) = 0 \Rightarrow P = Q$ (that is, $d_{\mathcal{F}}$ is a metric).
- assumptions required in order to ensure that $d_{\mathcal{F}} < +\infty$.

Some problems with the likelihood Minimum Distance Estimation (MDE)

Non-asymptotic bound for MDE

Theorem 1

- X_1, \ldots, X_n i.i.d from P_0 ,
- for any $f \in \mathcal{F}$, $\sup_{x \in \mathcal{X}} |f(x)| \leq 1$.

Then

$$\mathbb{E}\left[d_{\mathcal{F}}(P_{\hat{\theta}_{d_{\mathcal{F}}}},P_0)\right] \leq \inf_{\theta \in \Theta} d_{\mathcal{F}}(P_{\theta},P_0) + 4.\mathrm{Rad}_n(\mathcal{F})$$

Rademacher complexity

$$\operatorname{Rad}_n(\mathcal{F}) := \sup_{P} \mathbb{E}_{Y_1, \dots, Y_n \sim P} \mathbb{E}_{\epsilon_1, \dots, \epsilon_n} \left| \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \epsilon_i f(Y_i) \right|.$$

where $\epsilon_1, \ldots, \epsilon_n$ are i.i.d Rademacher variables :

$$\mathbb{P}(\epsilon_1 = 1) = \mathbb{P}(\epsilon_1 = -1) = 1/2.$$

Some problems with the likelihood Minimum Distance Estimation (MDE)

Example 1 : set of indicators

$$\mathbb{1}_{A}(x) = \begin{cases} 1 \text{ if } x \in A, \\ 0 \text{ if } x \notin A. \end{cases}$$

Image from Wikipedia.

- - -

3 points shattered



Reminder - Vapnik-Chervonenkis dimension

- Assume that $\mathcal{F} = \{\mathbb{1}_A, A \in \mathcal{A}\}$ for some $\mathcal{A} \subseteq \mathcal{P}(\mathcal{X})$,
 - $S_{\mathcal{F}}(x_1,...,x_n) := \{(f(x_1),...,f(x_n)), f \in \mathcal{F}\},$ • $VC(\mathcal{F}) := \max\{n : \exists x_1,...,x_n, |S_{\mathcal{F}}(x_1,...,x_n)| = 2^n\}.$

Theorem (Bartlett and Mendelson)

$$\operatorname{Rad}_n(\mathcal{F}) \leq \sqrt{\frac{2.\operatorname{VC}(\mathcal{F})\log(n+1)}{n}}$$

Bartlett, P. L. & Mendelson, S. (2002). Rademacher and Gaussian complexities : Risk bounds and structural results. *JMLR*.

Some problems with the likelihood Minimum Distance Estimation (MDE)

Example 1 : KS and TV distances

Two classical examples :

- $\mathcal{A} = \{ \text{all measurable sets in } \mathcal{X} \}$, then $d_{\mathcal{F}}(\cdot, \cdot)$ is the total variation distance $TV(\cdot, \cdot)$.
 - $\operatorname{VC}(\mathcal{F}) = +\infty$ when $|\mathcal{X}| = +\infty$,
 - in general, $\operatorname{Rad}_n(\mathcal{F}) \nrightarrow 0$.
- $\mathcal{X} = \mathbb{R}$, $\mathcal{A} = \{(-\infty, x], x \in \mathbb{R}\}$, then $d_{\mathcal{F}}(\cdot, \cdot)$ is the Kolmogorov-Smirnov distance $\mathrm{KS}(\cdot, \cdot)$.
 - KS distance was actually proposed by S. Holm for robust estimation,
 - $\operatorname{VC}(\mathcal{F}) = 1$.

$$\mathbb{E}\left[\mathrm{KS}(P_{\hat{\theta}_{\mathrm{KS}}}, P_0)\right] \leq \inf_{\theta \in \Theta} \mathrm{KS}(P_{\theta}, P_0) + 4.\sqrt{\frac{2\log(n+1)}{n}}.$$

Example 2 : Maximum Mean Discrepancy (MMD)

• Let $(\mathcal{H}, \langle \cdot, \cdot
angle_{\mathcal{H}})$ be a RKHS with kernel

$$k(x,y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}.$$

• If $\|\phi(x)\|_{\mathcal{H}} = k(x,x) \leq 1$ then $\mathbb{E}_{X \sim P}[\phi(X)]$ is well-defined .

• The map $P \mapsto \mathbb{E}_{X \sim P}[\phi(X)]$ is one-to-one if k is *characteristic*.

• For example,
$$k(x,y) = \exp(-\|x-y\|^2/\gamma^2)$$
 works.

Definition - MMD

$$\begin{split} \mathrm{MMD}_k(P,Q) &= \sup_{\substack{f \in \mathcal{H} \\ \|f\|_{\mathcal{H}} \leq 1}} \left\| \mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{X \sim Q}[f(X)] \right\| \\ &= \left\| \mathbb{E}_{X \sim P}[\phi(X)] - \mathbb{E}_{X \sim Q}[\phi(X)] \right\|_{\mathcal{H}}. \end{split}$$

Some problems with the likelihood Minimum Distance Estimation (MDE)

Example 2 : MMD

$$\mathcal{F} = \{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1\} \Rightarrow \operatorname{Rad}_n(\mathcal{F}) \leq \sqrt{\frac{\sup_x k(x,x)}{n}}$$

Theorem 2

For k bounded by 1 and characteristic,

$$\mathbb{E}\left[\mathrm{MMD}_{k}(P_{\hat{\theta}_{\mathrm{MMD}_{k}}},P_{0})\right] \leq \inf_{\theta \in \Theta} \mathrm{MMD}_{k}(P_{\theta},P_{0}) + \frac{2}{\sqrt{n}}$$



Joint work with Badr-Eddine Chérief-Abdellatif (Oxford).



Chérief-Abdellatif, B.-E. and Alquier, P. Finite Sample Properties of Parametric MMD Estimation : Robustness to Misspecification and Dependence. Bernoulli, 2022.

Some problems with the likelihood Minimum Distance Estimation (MDE)

Example 3 : Wasserstein

Another classical metric belongs to the IPS family :

$$W_{\delta}(P,Q) = \sup_{\substack{f: \mathcal{X} \to \mathbb{R} \\ \operatorname{Lip}(f) \leq 1}} \left| \mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{X \sim Q}[f(X)] \right|$$

where $\operatorname{Lip}(f) := \sup_{x \neq y} |f(x) - f(y)| / \delta(x, y).$

- In general, Rad_n(F) → 0, so will not converge in full generality as with MMD and KS.
- However, nice results can be proven under additional assumptions :

Bernton, E., Jacob, P. E., Gerber, M. & Robert, C. P. (2019). On parameter estimation with the Wasserstein distance. *Information and Inference : A Journal of the IMA*.

MDE and robustness : Huber's contamination

Reminder

$$\mathbb{E}\left[d_{\mathcal{F}}(P_{\hat{\theta}_{d_{\mathcal{F}}}},P_0)\right] \leq \inf_{\theta \in \Theta} d_{\mathcal{F}}(P_{\theta},P_0) + 4.\mathrm{Rad}_n(\mathcal{F}).$$

Huber's contamination model : $P_0 = (1 - \varepsilon)P_{\theta_0} + \varepsilon Q$.

$$d_{\mathcal{F}}(P_{\theta_{0}}, P_{0}) = \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{X \sim P_{\theta_{0}}} f(X) - (1 - \varepsilon) \mathbb{E}_{X \sim P_{\theta_{0}}} f(X) - \varepsilon \mathbb{E}_{X \sim Q} f(X) \right|$$

=
$$\sup_{f \in \mathcal{F}} \left| \varepsilon \mathbb{E}_{X \sim P_{\theta_{0}}} f(X) - \varepsilon \mathbb{E}_{X \sim Q} f(X) \right|$$

=
$$\varepsilon . d_{\mathcal{F}}(P_{\theta_{0}}, Q) \leq 2\varepsilon \quad \text{if for any } f \in \mathcal{F}, \sup_{x} |f(x)| \leq 1$$

Corollary - in Huber's contamination model

$$\mathbb{E}\left[d_{\mathcal{F}}(P_{\hat{\theta}_{d_{\mathcal{F}}}}, P_{\theta_0})\right] \leq 4\varepsilon + 4.\mathrm{Rad}_n(\mathcal{F}).$$

Some problems with the likelihood Minimum Distance Estimation (MDE)

MDE and robustness : toy experiment

Model : $\mathcal{N}(\theta, 1)$, X_1, \ldots, X_n i.i.d $\mathcal{N}(\theta_0, 1)$, n = 100 and we repeat the exp. 200 times. Kernel $k(x, y) = \exp(-|x - y|)$.

	$\hat{ heta}_{MLE}$	$\hat{ heta}_{ ext{MMD}_k}$	$\hat{ heta}_{\mathrm{KS}}$
mean abs. error	0.081	0.094	0.088

Now, $\varepsilon = 2\%$ of the observations drawn from a Cauchy.

 $\begin{array}{c} \text{mean abs. error} \quad 0.276 \quad 0.095 \quad 0.088\\ \text{Now, } \varepsilon = 1\% \text{ are replaced by } 1,000. \end{array}$

mean abs. error 10.008 0.088 0.082

Details on the computation of the MMD estimator Complex models

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Reminder

Details on the computation of the MMD estimator Complex models

$k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$, k bounded by 1 and characteristic.

Reminder - MMD

$$\begin{split} \mathrm{MMD}_k(P,Q) &= \sup_{f \in \mathcal{H} \\ \|f\|_{\mathcal{H}} \leq 1}} \left| \mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{X \sim Q}[f(X)] \right| \\ &= \left\| \mathbb{E}_{X \sim P}[\phi(X)] - \mathbb{E}_{X \sim Q}[\phi(X)] \right\|_{\mathcal{H}}. \end{split}$$

Details on the computation of the MMD estimator Complex models

More explicit formulas for the MMD

We actually have

$$\begin{split} \mathrm{MMD}_{k}^{2}(P_{\theta},\hat{P}_{n}) &= \mathbb{E}_{X,X'\sim P_{\theta}}[k(X,X')] - \frac{2}{n} \sum_{i=1}^{n} \mathbb{E}_{X\sim P_{\theta}}[k(X_{i},X)] \\ &+ \frac{1}{n^{2}} \sum_{1 \leq i,j \leq n} k(X_{i},X_{j}) \end{split}$$
and so

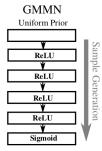
$$\nabla_{\theta} \text{MMD}_{k}^{2}(P_{\theta}, \hat{P}_{n})$$

$$= 2\mathbb{E}_{X, X' \sim P_{\theta}} \left\{ \left[k(X, X') - \frac{1}{n} \sum_{i=1}^{n} k(X_{i}, X) \right] \nabla_{\theta} [\log p_{\theta}(X)] \right\}$$

that can be approximated by sampling from P_{θ} .

Details on the computation of the MMD estimator Complex models

Generative Adversarial Networks (GAN, 1/2)



Generative model $X \sim P_{\theta}$:

- $U \sim \text{Unif}[0, 1]^d$,
- $X = F_{\theta}(U)$ where F_{θ} is some NN with weights θ .



Pierre Alquier, RIKEN AIP Minimum Distance Estimation

GAN (2/2)

Details on the computation of the MMD estimator Complex models

Results from Dziugaite et al. (2015).



Details on the computation of the MMD estimator Complex models

Inference for Systems of SDEs (1/2)



Briol, F. X., Barp, A., Duncan, A. B., & Girolami, M. (2019). Statistical Inference for Generative Models with Maximum Mean Discrepancy. *Preprint arXiv* :1906.05944.

$$\mathrm{d}X_t = b(X_t, \theta_1)\mathrm{d}t + \sigma(X_t, \theta_2)\mathrm{d}W_t$$

- easy to sample from the model with a given $\theta = (\theta_1, \theta_2)$,
- they propose a method to approximate the gradient of the MMD criterion.

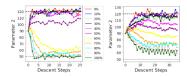
Details on the computation of the MMD estimator Complex models

Inference for Systems of SDEs (2/2)

Example in a (stochastic) Lotka-Volterra model.



Results from Briol et al. (2019) : compare MMD minimization to Wasserstein minimization.



Details on the computation of the MMD estimator $\ensuremath{\mathsf{Complex}}$ models

Regression

- problem with regression : we want to specify and estimate a parametric model P_{θ(X)} for Y|X. MMD requires to specify a model for (X, Y).
- natural idea : estimate the distribution of X by $\frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}$ and use the MMD procedure on $P_{\theta(X)}$.
- the previous theory shows directly that we estimate the distribution of (X, Y) consistently.
- it is far more difficult to prove that we estimate the distribution of Y|X.



Joint work with M. Gerber (Bristol).

Alquier, P. and Gerber, M. (2020). Universal Robust Regression via Maximum Mean Discrepancy. Preprint arXiv.

Copulas

- another semi-parametric model, MMD approach can be adapted.
- asymptotic theory + R package.

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Details on the computation of the MMD estimator

With B.-E. Chérief-Abdellatif (Oxford), J.-D. Fermanian (ENSAE Paris), A. Derumigny (TU Delft).

Alquier, P., Chérief-Abdellatif, B.-E., Derumigny, A. and Fermanian, J.-D. Estimation of copulas via Maximum Mean Discrepancy. JASA, to appear.



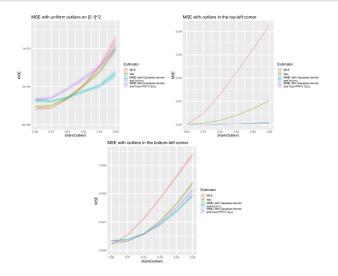




Complex models

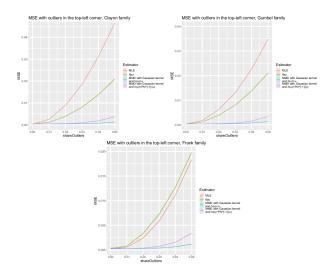
Details on the computation of the MMD estimator Complex models

Example : Gaussian copulas



Details on the computation of the MMD estimator Complex models

Example : other models



1st approach : "generalized posteriors" 2nd approach : ABC

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1st approach : "generalized posteriors" 2nd approach : ABC

Generalized posteriors

Posterior

$$\pi(\theta|X_1,\ldots,X_n)\propto L_n(\theta)\pi(\theta).$$

Generalized posterior

$$\hat{\pi}_{\beta,R_n}(\theta) \propto \exp(-\beta.R_n(\theta))\pi(\theta).$$

- old idea in ML (PAC-Bayes, forecasting with expert advice...) and in statistics (Gibbs posteriors...)
- popularized / extended and studied by :



Bissiri, P. G., Holmes, C. C. & Walker, S. G. (2016). A general framework for updating belief distributions. JRSS-B.

Knoblauch, J., Jewson, J. & Damoulas, T. (2022). An Optimization-centric View on Bayes' Rule : Reviewing and Generalizing Variational Inference. *JMLR* (to appear).

1st approach : "generalized posteriors" 2nd approach : ABC

Generalizing the posterior with IPS

Generalized posterior with IPS

$$\hat{\pi}_{\beta,R_n}(\theta) \propto \exp(-\beta.d_{\mathcal{F}}(P_{\theta},\hat{P}_n))\pi(\theta).$$

• in the MMD case : non-asymptotic result in

Chérief-Abdellatif, B.-E. and Alquier, P. (2020). MMD-Bayes : Robust Bayesian Estimation via Maximum Mean Discrepancy. *Proceedings of AABI*.

• computation via variational approximations.

1st approach : "generalized posteriors" 2nd approach : ABC

Reminder on ABC

Approximate Bayesian Computation (ABC)

input : sample $X_1^n = (X_1, \ldots, X_n)$, model $(P_{\theta}, \theta \in \Theta)$, prior π , statistic *S*, distance δ and threshold ϵ .

(i) sample
$$\theta \sim \pi$$
,
(ii) sample $Y_1^n = (Y_1, \dots, Y_n)$ i.i.d. from P_{θ}
• if $\delta(S(X_1^n), S(Y_1^n)) \leq \epsilon$ return θ ,
• else goto (i).

- how close is the distribution of the output to the posterior $\pi(\theta|X_1,\ldots,X_n)$?
- reverse point of view : what are the properties of the "generalized posterior" we sample from ?

1st approach : "generalized posteriors" 2nd approach : ABC

ABC with IPS

Here, we study the situation :

IPS-ABC

input : sample $X_1^n = (X_1, ..., X_n)$, model $(P_\theta, \theta \in \Theta)$, prior π , set of functions \mathcal{F} and threshold ϵ . Put $\hat{P}_n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$. (i) sample $\theta \sim \pi$, (ii) sample $Y_1^n = (Y_1, ..., Y_n)$ i.i.d. from P_θ and put $\hat{P}_n^Y = \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}$, • if $d_{\mathcal{F}}(\hat{P}_n, \hat{P}_n^Y) \leq \epsilon$ return θ , • else goto (i).

Notation : the output $\vartheta \sim \hat{\pi}_{n,\epsilon}^{\mathcal{F}}(\cdot)$.

1st approach : "generalized posteriors" 2nd approach : ABC

Properties of $\hat{\pi}_{n,\epsilon}^{\mathcal{F}}(\cdot)$

In a forthcoming joint paper with S. Legramanti (University of Bergamo) and D. Durante (Bocconi University, Milan) we study 3 questions :



$$\hat{\pi}_{n,\epsilon}^{\mathcal{F}}(\theta) \xrightarrow[\epsilon \searrow ?]{\epsilon \searrow ?} \pi(\theta | X_1^n).$$

$$\hat{\pi}_{n,\epsilon}^{\mathcal{F}}(\theta) \xrightarrow[n \to \infty]{} ?$$

$$\hat{\pi}_{n,\epsilon_n}^{\mathcal{F}}(\cdot) \xrightarrow[n \to \infty]{} \delta_{\theta_0} \text{ if } P_0 = P_{\theta_0}.$$

1st approach : "generalized posteriors" 2nd approach : ABC

Contraction of the ABC posterior

$$\epsilon_* := \inf_{\theta \in \Theta} d_{\mathcal{F}}(P_{\theta}, P_0).$$

Theorem 3

Assume :

- for all $\epsilon > 0$, $\pi(\{\theta : d_{\mathcal{F}}(P_{\theta}, P_0) \le \epsilon_* + \epsilon\}) \ge c\epsilon^d$.
- $\forall f \in \mathcal{F}$, $\sup_{x \in \mathcal{X}} |f(x)| \leq 1$.
- $\operatorname{Rad}_n(\mathcal{F}) \xrightarrow[n \to \infty]{} 0.$

Let ϵ_n be any sequence such that $\epsilon_n/\operatorname{Rad}_n(\mathcal{F}) \to \infty$ and $n\epsilon_n^2 \to \infty$. Then, with probability $\to 1$ on the sample, for any $M_n \to \infty$,

$$\hat{\pi}_{n,\epsilon_*+\epsilon_n}^{\mathcal{F}}\left(d_{\mathcal{F}}(P_{\theta},P_0) \leq \epsilon_* + \frac{4\epsilon_n}{3} + \operatorname{Rad}_n(\mathcal{F}) + \sqrt{\frac{\log\frac{M_n}{\epsilon_n^d}}{n}}\right) \geq 1 - \frac{2.3^d}{cM_n}.$$

1st approach : "generalized posteriors" 2nd approach : ABC

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終わり ありがとう ございます。