Concentration and robustness of discrepancy-based ABC

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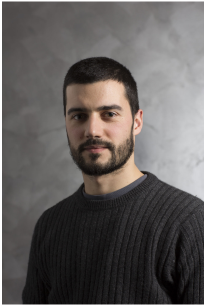

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Contents

Estimators, randomized estimators and Bayes rule

- $Y_{1:n} = Y_1, \ldots, Y_n$ i.i.d from μ^*,
- model : $(\mu_\theta, \theta \in \Theta)$,
- estimator : $\hat{\theta} = \hat{\theta}(Y_{1:n})$,
- randomized estimator : $\hat{\rho}(\cdot) = \hat{\rho}(Y_{1:n})(\cdot)$ probability measure on Θ.

Examples of randomized estimators :

- posterior : $\hat{\rho}(\theta) = \pi(\theta | Y_{1:n}) \propto \underbrace{\mathcal{L}(\theta; Y_{1:n})}_{\text{likelihood}} \underbrace{\pi(\theta)}_{\text{prior}}$,
- fractional/tempered posterior : $\hat{\rho}(\theta) \propto [\mathcal{L}(\theta; Y_{1:n})]^\alpha \pi(\theta)$,
- Gibbs estimator : $\hat{\rho}(\theta) \propto \exp[-\eta \underbrace{R(\theta; Y_{1:n})}_{\text{loss}}]\pi(\theta)$.

Evaluating randomized estimators

Assume in this slide that $\mu^* = \mu_{\theta_0}$: "the truth is in the model".

Statistical performance of an estimator :

- consistency : $d(\hat{\theta}, \theta_0) \xrightarrow[n\to\infty]{} 0$ (in proba., a.s., ...) ?
- rate of convergence : $\mathbb{E}_{Y_{1:n}}[d(\hat{\theta}, \theta_0)] \leq r_n \xrightarrow[n\to\infty]{} \theta_0$?
- ...

For a randomized estimator :

- contraction rate :

$$\mathbb{P}_{\theta\sim\hat{\rho}}[d(\theta, \theta_0) \geq r_n] \xrightarrow[n\to\infty]{} 0 \text{ (in proba., a.s., ...) ?}$$

- average risk : $\mathbb{E}_{Y_{1:n}}\left[\mathbb{E}_{\theta\sim\hat{\rho}}[d(\theta, \theta_0)]\right] \leq r_n$?
- ...

Approximate Bayesian Inference

- Well-known conditions to prove contraction of the posterior,
- tools from ML for randomized estimators : PAC-Bayes bounds.

Given a "non-exact" algorithm targetting $\hat{\rho}$ instead of $\pi(\cdot|Y_{1:n})$: variational approximations, ABC, etc., we can

- quantify how well $\hat{\rho}$ approximates $\pi(\cdot|Y_{1:n})$?
- study $\hat{\rho}$ as a randomized estimator and study its contraction/convergence.

Contents

Reminder on ABC

Approximate Bayesian Computation (ABC)

INPUT : sample $Y_{1:n} = (Y_1, \dots, Y_n)$, model $(\mu_\theta, \theta \in \Theta)$, prior π, statistic S, metric δ and threshold ϵ.

(i) sample $\theta \sim \pi$,

(ii) sample $Z_{1:n} = (Z_1, \dots, Z_n)$ i.i.d. from P_θ :

- if $\delta(S(Y_{1:n}), S(Z_{1:n})) \leq \epsilon$ return θ,
- else goto (i).

OUTPUT : $\vartheta \sim \hat{\rho}$.

- discrete sample space, if S =identity and $\epsilon = 0$, ABC is actually exact : $\hat{\rho}(\cdot) = \pi(\cdot|Y_{1:n})$.
- general case : ABC not exact, we can ask two questions :
  1. is $\hat{\rho}(\cdot)$ a good approximation of $\pi(\cdot|Y_{1:n})$?
  2. is $\hat{\rho}$ a good randomized estimator ?

Reminder on IPM

Integral Probability Metrics (IPM)

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

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

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

In general, only a semimetric. However, in many cases, it is actually a metric : $d_{\mathcal{F}}(\mu,\nu) = 0 \Rightarrow \mu = \nu$. Examples :

- total variation : $\mathcal{F} = \{1_A,\ A \text{ measurable}\}$,
- Kolmogorov : $\mathcal{F} = \{1_{(-\infty,x]},\ x \in \mathbb{R}\}$,
- Wasserstein : $\mathcal{F}$ = set of 1-Lipschitz functions,
- Dudley...

Example : Maximum Mean Discrepancy (MMD)

- RKHS $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ with kernel $k(x,y) = \langle\phi(x),\phi(y)\rangle_{\mathcal{H}}$.
- If $\|\phi(x)\|_{\mathcal{H}} = k(x,x) \leq 1$ then $\mathbb{E}_{X\sim\mu}[\phi(X)]$ is well-defined .
- The map $P \mapsto \mathbb{E}_{X\sim\mu}[\phi(X)]$ is one-to-one if k is characteristic.
- Gaussian kernel $k(x,y) = \exp(-\|x-y\|^2/\gamma^2)$ satisfies these assumption.

$$\mathcal{F} = \{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1\}.$$

$$\begin{aligned} d_{\mathcal{F}}(\mu,\nu) &= \sup_{f\in\mathcal{F}} \left| \mathbb{E}_{X\sim\mu}[f(X)] - \mathbb{E}_{X\sim\nu}[f(X)] \right| \\ &= \left\| \mathbb{E}_{X\sim\mu}[\phi(X)] - \mathbb{E}_{X\sim\nu}[\phi(X)] \right\|_{\mathcal{H}}. \end{aligned}$$

IPM and statistical estimation

We define the "empirical probability distribution"

$$\hat{\mu}_{Y_{1:n}} := \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}.$$

Minimum distance estimator

$$\hat{\theta} := \arg\min_{\theta \in \Theta} d_{\mathcal{F}} \left(\mu_\theta, \hat{\mu}_{Y_{1:n}} \right).$$

Theorem

If $d_{\mathcal{F}}$ is the MMD for a bounded & characteristic kernel,

$$\mathbb{E} \left[d_{\mathcal{F}}(\mu_{\hat{\theta}}, \mu^*) \right] \leq \inf_{\theta \in \Theta} d_{\mathcal{F}}(\mu_\theta, \mu^*) + \frac{2}{\sqrt{n}}.$$

Robust estimation with MMD

$$\mathbb{E}\left[d_{\mathcal{F}}(\mu_{\hat{\theta}}, \mu^*)\right] \leq \inf_{\theta \in \Theta} d_{\mathcal{F}}(\mu_\theta, \mu^*) + \frac{2}{\sqrt{n}}.$$

- well-specified case, $\mu^* = \mu_{\theta_0}$,

$$\mathbb{E}\left[d_{\mathcal{F}}(\mu_{\hat{\theta}}, \mu_{\theta_0})\right] \leq 2/\sqrt{n}.$$

- Huber contamination model $\mu^* = (1-\varepsilon)\mu_{\theta_0} + \varepsilon\nu$,

$$\begin{aligned} d_{\mathcal{F}}(\mu_{\theta_0}, \mu^*) &= \sup_{f \in \mathcal{F}} \left|\mathbb{E}_{X\sim\mu_{\theta_0}} f(X) - (1-\varepsilon)\mathbb{E}_{X\sim\mu_{\theta_0}} f(X) - \varepsilon\mathbb{E}_{X\sim\nu} f(X)\right| \\ &= \varepsilon \sup_{f \in \mathcal{F}} \left|\mathbb{E}_{X\sim\mu_{\theta_0}} f(X) - \mathbb{E}_{X\sim\nu} f(X)\right| \leq 2\varepsilon \end{aligned}$$

$$\mathbb{E}\left[d_{\mathcal{F}}(\mu_{\hat{\theta}}, \mu_{\theta_0})\right] \leq 4\varepsilon + 2/\sqrt{n}.$$

MDE and robustness : toy experiment

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

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

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

mean abs. error	0.276	0.095	0.088

Now, $\varepsilon = 1\%$ are replaced by $1,000$.

mean abs. error	10.008	0.088	0.082

References on minimum MMD estimation

Dziugaite, G. K., Roy, D. M., & Ghahramani, Z. (2015). Training generative neural networks via maximum mean discrepancy optimization. UAI 2015.

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

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

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

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

Contents

Discrepancy-based ABC

Approximate Bayesian Computation (ABC)

INPUT : sample $Y_{1:n}$, model $(\mu_\theta, \theta \in \Theta)$, prior π, IPM $d_{\mathcal{F}}$ and threshold ϵ.

(i) sample $\theta \sim \pi$,

(ii) sample $Z_{1:n}$ i.i.d. from P_θ :

- if $d_{\mathcal{F}}(\hat{\mu}_{Y_{1:n}}, \hat{\mu}_{Z_{1:n}}) \leq \epsilon$ return θ,
- else goto (i).

OUTPUT : $\vartheta \sim \hat{\rho}_\epsilon$.

Rermark : when $d_{\mathcal{F}}$ is the MMD with kernel k,

$$d_{\mathcal{F}}(\hat{\mu}_{Y_{1:n}}, \hat{\mu}_{Z_{1:n}}) = \sum_{i,j} k(Y_i, Y_j) - 2 \sum_{i,j} k(Y_i, Z_j) + \sum_{i,j} k(Z_i, Z_j).$$

Approximation of the posterior

Bernton, E., Jacob, P. E., Gerber, M. & Robert, C. P. (2019). Approximate Bayesian Computation with the Wasserstein distance. JRSS-B.

Contains a general result that can be applied here.

Theorem

Assume

- μ_θ has a continuous density f_θ and for some neighborhood V of $Y_{1:n}$ we have $\sup_{\theta\in\Theta}\sup_{v_{1:n}\in V}\prod_{i=1}^{n} f_\theta(v_i) < +\infty$.
- $v_{1:n} \mapsto d_{\mathcal{F}}(\hat{\mu}_{Y_{1:n}}, \hat{\mu}_{v_{1:n}})$ is continuous.

Then

$$\forall \text{ measurable set } A,\ \hat{\rho}_\epsilon(A) \xrightarrow[\epsilon\to 0]{} \pi(A|Y_{1:n}).$$

Assumptions for contraction

(C1) $\mathcal{Y}$-valued $Y_{1:n} = (Y_1, \dots, Y_n)$ i.i.d from μ_*, put :

$$\epsilon^* := \inf_{\theta \in \Theta} d_{\mathcal{F}}(\mu_\theta, \mu_*).$$

(C2) prior mass condition : there is $c > 0, L \geq 1$ such that

$$\pi\left(\left\{ \theta \in \Theta : d_{\mathcal{F}}(\mu_\theta, \mu_*) - \epsilon^* \leq \epsilon \right\} \right) \geq c\epsilon^L$$

(C3) functions in $\mathcal{F}$ are bounded :

$$\sup_{f \in \mathcal{F}} \sup_{y \in \mathcal{Y}} |f(y)| \leq b.$$

(C4) the Rademacher complexity $\mathfrak{R}_n(\mathcal{F})$ satisfies

$$\mathfrak{R}_n(\mathcal{F}) \xrightarrow[n \to \infty]{} 0.$$

Reminder on Rademacher complexity

Rademacher complexity

$$\mathfrak{R}_n(\mathcal{F}) := \sup_{\mu} \mathbb{E}_{Y_1,\dots,Y_n\sim\mu} \mathbb{E}_{\varepsilon_1,} \text{R}\mathit{ESULTATDEFUKUMIZUACITER,ESTIMATIONET}$$

where $\varepsilon_1, \dots, \varepsilon_n$ are i.i.d Rademacher variables :

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

Examples

- TV : $\mathcal{F} = \{1_A,\ A \text{ measurable}\}$,

$$\mathfrak{R}_n(\mathcal{F}) \nrightarrow 0 \text{ in general.}$$

- Kolmogorov : $\mathcal{F} = \{1_{(-\infty,x]},\ x \in \mathbb{R}\}$,

$$\mathfrak{R}_n(\mathcal{F}) \leq 2\sqrt{\frac{\log(n+1)}{n}} \to 0.$$

- Wasserstein : $\mathcal{F} =$ set of 1-Lipschitz functions,

$$\mathfrak{R}_n(\mathcal{F}) \to 0 \text{ if } \mathcal{X} \text{ is bounded, see Corollary 8 in}$$

Sriperumbudur, B.K., Fukumizu, K., Gretton, A., Schölkopf, B., Lanckriet, G.R. (2010). Non-parametric estimation of integral probability metrics. IEEE International Symposium on Information Theory.

- MMD :

$$\mathfrak{R}_n(\mathcal{F}) \leq \sqrt{\frac{\sup_{y\in\mathcal{Y}} k(y,y)}{n}}.$$

Contraction of discrepancy-based ABC

Theorem 1

Under (C1)-(C4), with $\epsilon := \epsilon_n = \epsilon^* + \bar{\epsilon}_n$ with $\bar{\epsilon}_n \to 0$, $n\bar{\epsilon}_n^2 \to \infty$ and $\bar{\epsilon}_n / \mathfrak{R}_n(\mathcal{F}) \to \infty$. Then, for any sequence $M_n > 1$,

$$\hat{\rho}_{\epsilon_n}\left(\left\{\theta \in \Theta : d_{\mathcal{F}}(\mu_\theta, \mu_*) > \epsilon^* + r_n\right\}\right) \leq \frac{2 \cdot 3^L}{cM_n}$$

$$\text{where } r_n = \frac{4\bar{\epsilon}_n}{3} + 2\mathfrak{R}_n(\mathfrak{F}) + b\sqrt{\frac{2\log(\frac{M_n}{\bar{\varepsilon}_n^L})}{n}},$$

with probability $\to 1$ with respect to the sample $Y_{1:n}$.

Examples

- Assume $\mathfrak{R}_n(\mathcal{F}) \leq c\sqrt{1/n}$ (MMD, Kolmogorov...). Take $M_n = n$ and $\bar{\epsilon}_n = \sqrt{\log(n)/n}$ to get

$$\hat{\rho}_{\epsilon_n}\left(\left\{\theta \in \Theta : d_{\mathcal{F}}(\mu_\theta, \mu_*) > \epsilon^* + r_n\right\}\right) \leq \frac{2 \cdot 3^L}{cn}$$

where $r_n = \mathcal{O}\left(\sqrt{\log(n)/n}\right)$.

- Larger $\mathfrak{R}_n(\mathcal{F})$ will lead to slower rates.

Removing (C3)-(C4)

- if we remove (C3)-(C4), we cannot use classical concentration results on $d_{\mathcal{F}}(\mu_*, \hat{\mu}_{Y_{1:n}})$ and $d_{\mathcal{F}}(\mu_\theta, \hat{\mu}_{Z_{1:n}})$.
- we can still provide a result under the assumption that "some concentration holds", as

Bernton, E., Jacob, P. E., Gerber, M. & Robert, C. P. (2019). Approximate Bayesian Computation with the Wasserstein distance. JRSS-B.

for the Wasserstein distance.

- however, this will impose assumptions on μ_*, $\{\mu_\theta, \theta \in \Theta\}$ and might lead to slower contraction rates. In our paper, we illustrate this with MMD with unbounded kernels :

$$\mathfrak{R}_n(\mathcal{F}) \leq \sqrt{\frac{\sup_{y\in\mathcal{Y}} k(y,y)}{n}} = +\infty.$$

Example : MMD-ABC with unbounded kernel

Theorem 2

Under (C1)-(C2), and

(C5) $\mathbb{E}_{Y\sim\mu_*}[k(Y,Y)] < +\infty$,

(C6) $\sup_{\theta\in\Theta}\mathbb{E}_{Z\sim\mu_\theta}[k(Z,Z)] < +\infty$,

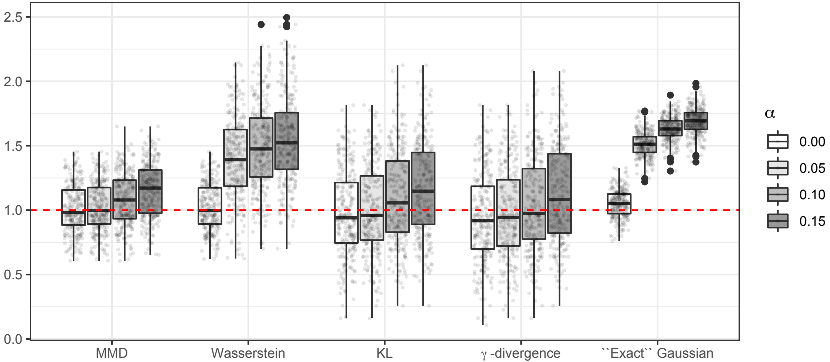
$\epsilon_n = \epsilon^* + \bar{\epsilon}_n$ with $\bar{\epsilon}_n \to 0$. Then, for some $C > 0$, for any sequence $M_n > 1$, with proba. $\to 1$,

$$\hat{\rho}_{\epsilon_n}\left(\left\{\theta\in\Theta : d_{\mathcal{F}}(\mu_\theta,\mu_*) > \epsilon^* + r_n\right\}\right) \leq \frac{C}{M_n}$$

$$\text{where } r_n = \frac{4\bar{\epsilon}_n}{3} + \frac{M_n^2}{n^2\bar{\epsilon}^{2L}}.$$

For example $M_n = \sqrt{n}$ we can get $r_n = \mathcal{O}(1/n^{2L+1})$.

Experiments in the Gaussian case



Conclusion

- we provide an analysis of discrepancy-based ABC for a large class of IPM.
- in particular, ABC with MMD leads to robust estimation, without assumptions on the model nor on the truth.
- note that other discrepancies were studied and probably more should be investigated

Frazier, D. T. (2020). Robust and efficient Approximate Bayesian Computation : A minimum distance approach. Preprint arXiv.

Nguyen, H. D., Arbel, J., Lü, H. and Forbes, F. (2020). Approximate Bayesian computation via the energy statistic. IEEE Access.

- important extension to non i.i.d observations (time series, etc.). Note that strong concentration of $d_{\mathcal{F}}\left(\mu_*, \hat{\mu}_{Y_{1:n}}\right)$ is known in this setting (our joint paper with B.-E. Chérief-Abdellatif, Bernoulli 2022).

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終わり

ありがとう ございます。