THE UNIVERSITY OF WARWICK

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Robust Bayesian Inference for Simulator-based Models via the MMD Posterior Bootstrap

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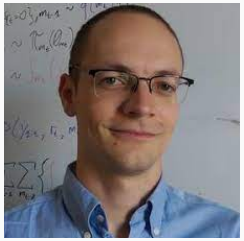

One World ABC seminar, May 25 2022

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Motivation

Simulator-based models

- Independent sampling is possible, but likelihood is unavailable
- Model is usually at best a rough approximation of a complex physical or biological phenomenon
- It will most likely not capture all of the key characteristics of the underlying data generating process.

Two main problems:

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Problem setting

Simulator-based model family

$$\mathcal{P}_\Theta = \{\mathbb{P}_\theta : \theta \in \Theta\} \subseteq \mathcal{P}$$

$\mathbb{P}_\theta$ is associated with *simulator* function $G_\theta : \mathcal{U} \to \mathcal{X}$ and probability measure $\mathbb{U}$ in space $\mathcal{U}$

$$y := G_\theta(u) \sim \mathbb{P}_\theta, u \sim \mathbb{U}.$$

Observed i.i.d. data $x_{1:n} \sim \mathbb{P}^*$

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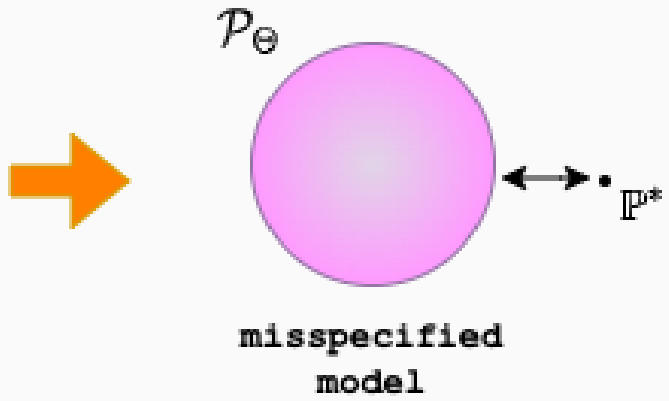

Background

Bayesian Nonparametric Learning (NPL) framework (Lyddon et al., 2018; Fong et al., 2019)

1. Place a nonparametric prior *directly* on the data-generating mechanism

$$\mathbb{P} \sim DP(\alpha, \mathbb{F}), \quad \mathbb{P}|x_{1:n} \sim DP\left(\alpha', \mathbb{F}'\right)$$

where

$$\alpha' = \alpha + n, \quad \mathbb{F}' := \frac{\alpha}{\alpha+n}\mathbb{F} + \frac{n}{n+\alpha}\mathbb{P}_n, \quad \mathbb{P}_n = \frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}$$

2. For a loss function $l(x, \theta)$ *propagate uncertainty* from $\mathbb{P}^*$ to the parameter of interest θ through

$$\boxed{\theta_l^*(\mathbb{P}^*) := \arg\inf_{\theta\in\Theta} \mathbb{E}_{X\sim\mathbb{P}^*}[l(X, \theta)]}$$

3. The push-forward measure $(\theta_l^*)_{\#}(\mathrm{DP}(\alpha', \mathbb{F}'))$ gives a posterior on Θ denoted by Π_{NPL}.

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Push-forward measure

To obtain independent realisations from Π_{NPL} at iteration j:

1. Sample $\mathbb{P}^{(j)}$ from the posterior DP;
2. Compute $\theta^{(j)} = \theta_I^*(\mathbb{P}^{(j)})$

Reminder:

Definition 2.1: Push-froward measure

Given measurable spaces (X_1, Σ_1) and (X_2, Σ_2), a measurable mapping $f : X_1 \to X_2$ and a measure $\mu : \Sigma_1 \to [0, +\infty]$, the pushforward of μ is defined to be the measure $f_{\#}(\mu) : \Sigma_2 \to [0, +\infty]$ given by

$$f_{\#}(\mu)(A) = \mu(f^{-1}(A)) \quad \text{for} \quad A \in \Sigma_2$$

Method

Distance-based loss function

$$\theta_l^*(\mathbb{P}^*) := \arg\inf_{\theta\in\Theta} \mathbb{E}_{X\sim\mathbb{P}^*}[l(X,\theta)]$$

$$\downarrow$$

$$\mathrm{D}(\mathbb{P}_\theta, \mathbb{P}^*)$$

- Use a distance-based loss between real and target distribution
- Target: $\theta_0 = \arg\inf_{\theta\in\Theta} D(\mathbb{P}^*, \mathbb{P}_\theta)$ for some distance function $D : \mathcal{P} \times \mathcal{P} \to \mathbb{R}_+$
- Minimisation of expected loss $\longrightarrow$ Minimum Distance Estimation (MDE), Parr and Schucany (1980)

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Proposal: Maximum Mean Discrepancy (MMD) based loss

- Proposal: *Maximum Mean Discrepancy (MMD)*
- Map θ^* now corresponds to a minimum MMD estimator as in Briol et al. (2019); Chérief-Abdellatif and Alquier (2022)
- *Integral Probability Metrics (IPMs), Müller (1997)*:

$$D(\mathbb{P}, \mathbb{Q}) = \sup_{f \in \mathcal{F}} \left| \int_{\mathcal{X}} f(x)\mathbb{P}(dx) - \int_{\mathcal{X}} f(x)\mathbb{Q}(dx) \right|$$

- **Maximum Mean Discrepancy (MMD)**: Restrict $\mathcal{F}$ to a unit *Reproducing Kernel Hilbert space* (RKHS), $\mathcal{H}_k$, defined through a symmetric, positive definite kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, with associated norm $\|\cdot\|_{\mathcal{H}_k}$ and inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_k} : \mathcal{H}_k \times \mathcal{H}_k \to \mathbb{R}$.
- Reproducing property:

$$f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}_k}$$

- Functions in $\mathcal{H}_k$ have the form $f(x) = \sum_{i=1}^{d} c_i k(x, x_i)$ for some $c_i \in \mathbb{R}$

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Maximum Mean Discrepancy (MMD)

- So MMD is defined as:

$$MMD(\mathbb{P},\mathbb{Q}) = \sup_{\substack{f\in\mathcal{H}_k,\\ \|f\|_{\mathcal{H}_k}\leq 1}} \left| \int_{\mathcal{X}} f(x)\mathbb{P}(dx) - \int_{\mathcal{X}} f(x)\mathbb{Q}(dx) \right|$$

- The MMD between two probability measures $\mathbb{P}$ and $\mathbb{Q}$ can be expressed as

$$\begin{aligned} MMD^2(\mathbb{P},\mathbb{Q}) := &\int_{\mathcal{X}}\int_{\mathcal{X}} k(x,y)\mathbb{P}(dx)\mathbb{P}(dy) - 2\int_{\mathcal{X}}\int_{\mathcal{X}} k(x,y)\mathbb{P}(dx)\mathbb{Q}(dy) \\ &+ \int_{\mathcal{X}}\int_{\mathcal{X}} k(x,y)\mathbb{Q}(dx)\mathbb{Q}(dy) \end{aligned}$$

- It can be estimated for example using a U-statistic as in Gretton et al. (2008):

$$\begin{aligned} MMD^2_{k,U}(\mathbb{P}^m,\mathbb{Q}^n) = &\frac{1}{m(m-1)}\sum_{i\neq j} k(y_i,y_j) - \frac{2}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m} k(x_i,y_j) \\ &+ \frac{1}{n(n-1)}\sum_{i\neq j} k(x_i,x_j) \end{aligned}$$

where $\{y_j\}_{j=1}^m \overset{iid}{\sim} \mathbb{P}$ and $\{x_i\}_{i=1}^n \overset{iid}{\sim} \mathbb{Q}$.

$$\longrightarrow \theta^*(\mathbb{P}^*) = \arg\inf_{\theta\in\Theta} \mathrm{MMD}^2_{k,U}(\mathbb{P}^*,\mathbb{P}_\theta)$$

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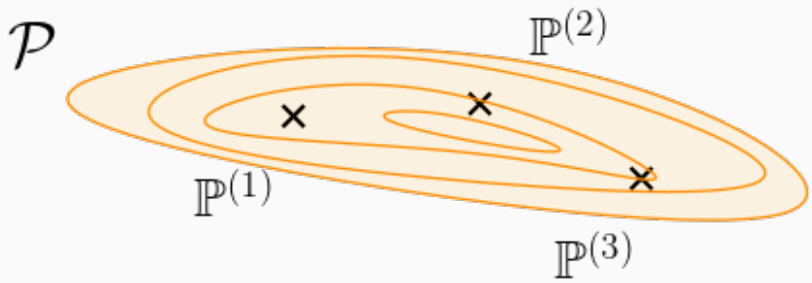
MMD Posterior Bootstrap

$$\mathbb{P}^{(1)}, \mathbb{P}^{(2)}, \mathbb{P}^{(3)} \overset{\text{iid}}{\sim} \mathrm{DP}(\alpha', \mathbb{F}')$$



1. Draw $\mathbb{P}^{(j)} \sim DP(\alpha', \mathbb{F}')$
2. Obtain $\theta^{(j)} := \theta^*(\mathbb{P}^{(j)}) = \arg\min_{\theta \in \Theta} \mathrm{MMD}^2_{k,U}(\mathbb{P}^{(j)}, \mathbb{P}_\theta)$

$$\tilde{x}^{(j)}_{1:T} \overset{\text{iid}}{\sim} \mathbb{F}, \quad (w^{(j)}_{1:n}, \tilde{w}^{(j)}_{1:T}) \sim \mathrm{Dir}\left(1, \ldots, 1, \frac{\alpha}{T}, \ldots, \frac{\alpha}{T}\right).$$

$$\mathbb{P}^{(j)} = \sum_{i=1}^{n} w_i^{(j)} \delta_{x_i} + \sum_{k=1}^{T} \tilde{w}_k^{(j)} \delta_{\tilde{x}_k^{(j)}} \sim \hat{\nu}. \tag{1}$$

where $\hat{\nu}$ denotes the probability measure on $\mathcal{P}$ defined by (1).

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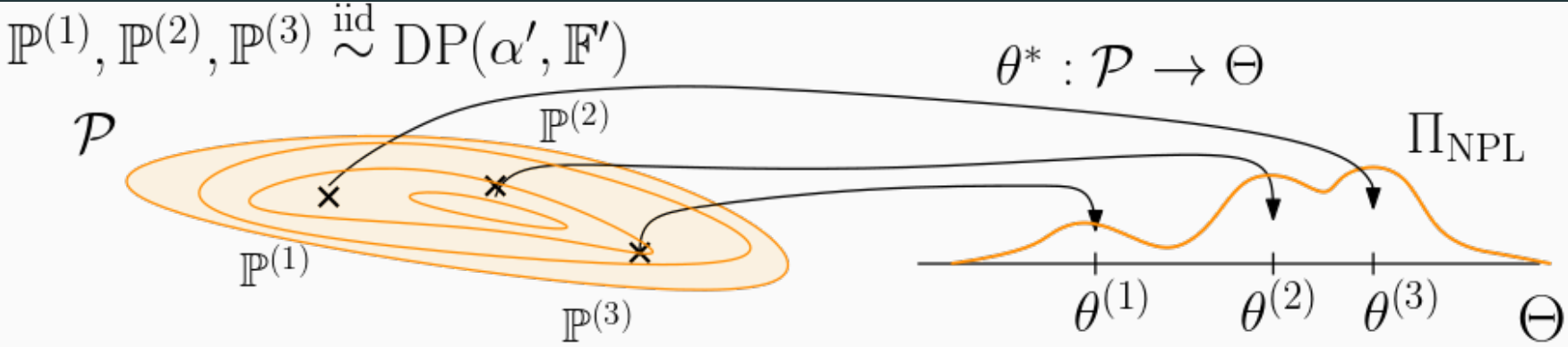

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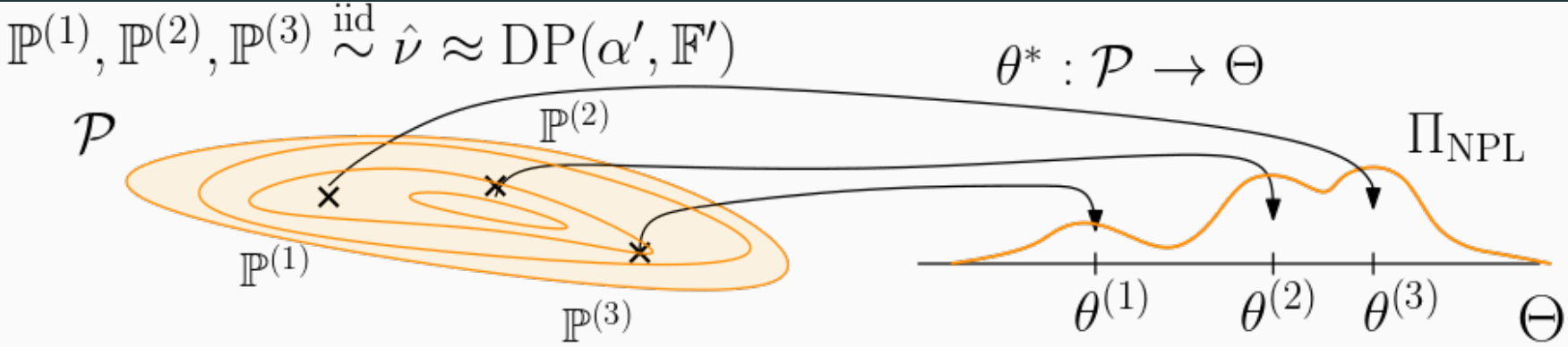

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Posterior Bootstrap with the MMD

Algorithm 1: MMD Posterior Bootstrap

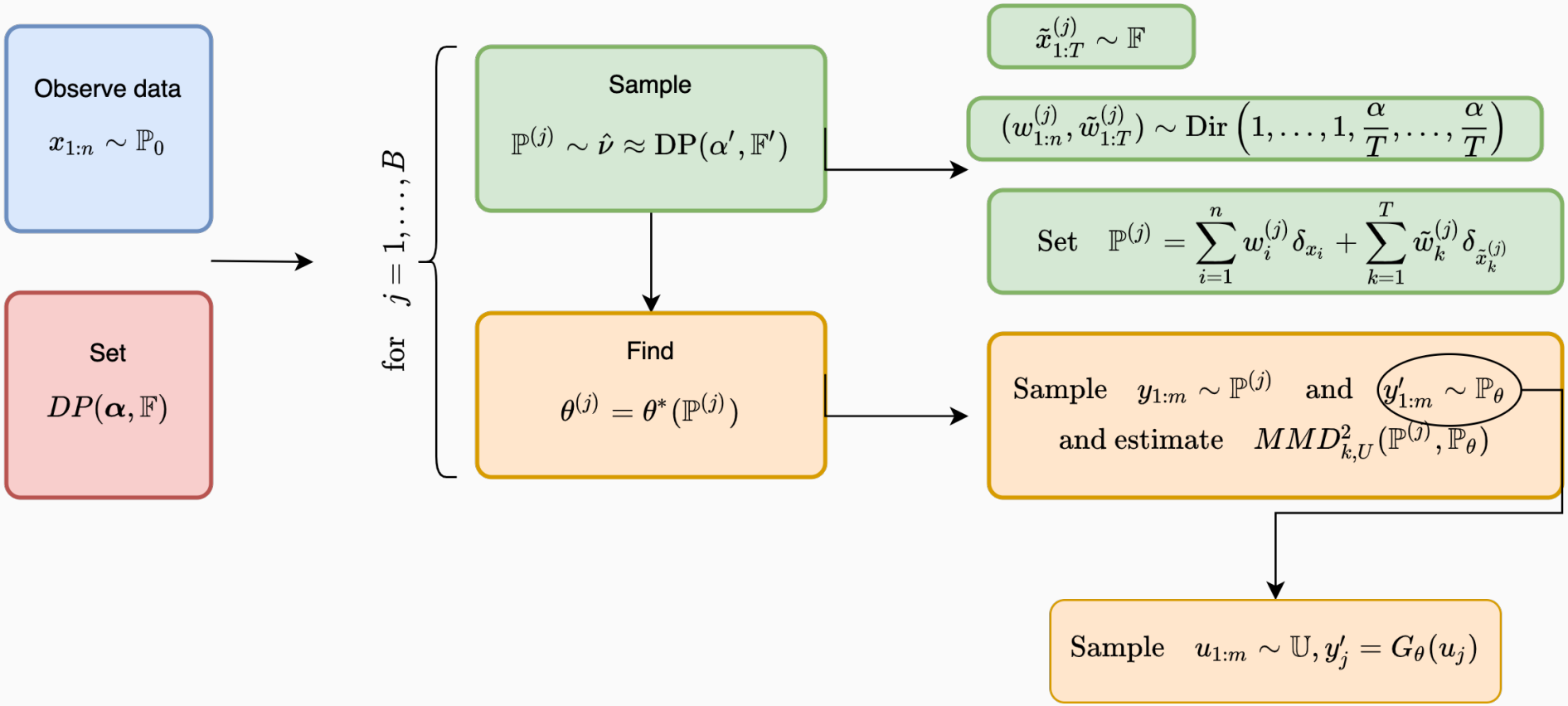
input: $x_{1:n}$, T, B, α, $\mathbb{F}$, $\mathbb{U}$, G_θ.

for $j \leftarrow 1$ **to** B **do**

- Sample $\tilde{x}_{1:T}^{(j)} \overset{\text{iid}}{\sim} \mathbb{F}$ and
- $(w_{1:n}^{(j)}, \tilde{w}_{1:T}^{(j)}) \sim \text{Dir}\left(1, \ldots, 1, \frac{\alpha}{T}, \ldots, \frac{\alpha}{T}\right)$.
- Set $\mathbb{P}^{(j)} = \sum_{i=1}^{n} w_i^{(j)} \delta_{x_i} + \sum_{k=1}^{T} \tilde{w}_k^{(j)} \delta_{\tilde{x}_k^{(j)}}$.
- Obtain $\theta^{(j)} = \theta^*(\mathbb{P}^{(j)})$ using numerical optimisation.

return Posterior bootstrap sample $\theta^{(1:B)}$

Posterior bootstrap with the MMD



Theoretical Results

Generalisation error

- **Assumption:** $\sup_{x,x' \in \mathcal{X}} |k(x, x')| < \infty$
- W.L.O.G. $|k(x, x')| \leq 1 \quad \forall \quad x, x' \in \mathcal{X}$

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$$\mathbb{E}_{x_{1:n} \overset{\text{iid}}{\sim} \mathbb{P}^*} \left[\mathbb{E}_{\mathbb{P} \sim \hat{\nu}} \left[\text{MMD}(\mathbb{P}^*, \mathbb{P}_{\theta^*(\mathbb{P})}) \right] \right]$$

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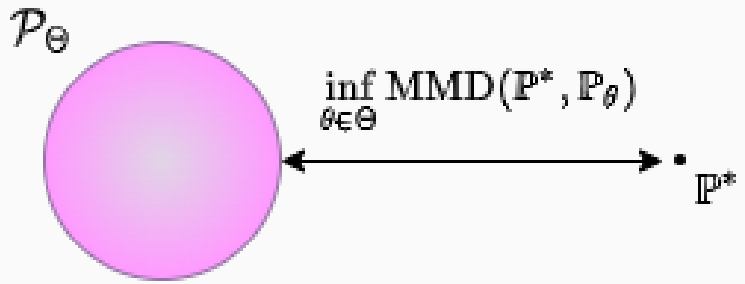
$$\inf_{\theta \in \Theta} \mathrm{MMD}(\mathbb{P}^*, \mathbb{P}_\theta) \quad \leq \quad \mathbb{E}_{x_{1:n} \overset{\text{iid}}{\sim} \mathbb{P}^*} \left[\mathbb{E}_{\mathbb{P} \sim \hat{\nu}} \left[\mathrm{MMD}(\mathbb{P}^*, \mathbb{P}_{\theta^*(\mathbb{P})}) \right] \right]$$



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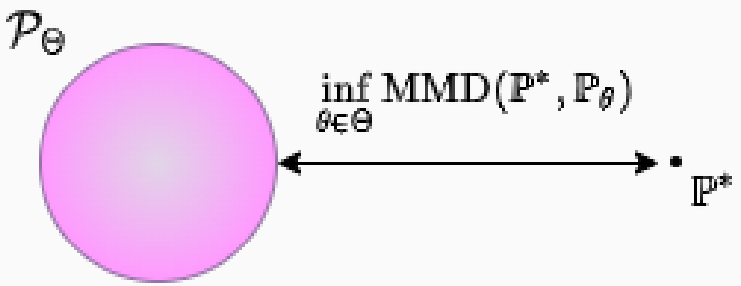
$$0 \leq \overbrace{\mathbb{E}_{x_{1:n} \overset{\text{iid}}{\sim} \mathbb{P}^*} \left[\mathbb{E}_{\mathbb{P} \sim \hat{\nu}} \left[\text{MMD}(\mathbb{P}^*, \mathbb{P}_{\theta^*(\mathbb{P})}) \right] \right] - \inf_{\theta \in \Theta} \text{MMD}(\mathbb{P}^*, \mathbb{P}_\theta)}^{\text{Generalisation Error}}$$

$$\leq \frac{2}{\sqrt{n}} + \frac{4\sqrt{\alpha(1+\alpha)}}{\sqrt{(\alpha+n)(\alpha+n+1)}}$$



- Rate agrees with results in Chérief-Abdellatif and Alquier (2022)

Posterior consistency

- For standard Bayesian inference with posterior measure Π_n defined on Θ directly, for any $M_n \to +\infty$ such that $M_n n^{-\frac{1}{2}} \to 0$:

$$\Pi_n \left(\theta \in \Theta : \mathrm{MMD}(\mathbb{P}_\theta, \mathbb{P}^*) > \inf_{\theta \in \Theta} \mathrm{MMD}(\mathbb{P}_\theta, \mathbb{P}^*) + \frac{M_n}{n^{1/2}} \right) \overset{n \to \infty}{\longrightarrow} 0 \tag{2}$$

- In our case:

$$\hat{\nu} \left(\mathbb{P} \in \mathcal{P} : \mathrm{MMD}(\mathbb{P}_{\theta^*(\mathbb{P})}, \mathbb{P}^*) > \inf_{\theta \in \Theta} \mathrm{MMD}(\mathbb{P}_\theta, \mathbb{P}^*) + \frac{M_n}{n^{1/2}} \right) \overset{n \to \infty}{\longrightarrow} 0.$$

Reminder: $\hat{\nu}$ is the approximation of the posterior $\mathrm{DP}(\alpha', \mathbb{F}')$

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Robustness to outliers

- Suppose $\mathbb{P}^* = (1-\epsilon)\tilde{\mathbb{P}} + \epsilon\,\mathbb{Q}$
- Then

$$\mathbb{E}_{x_{1:n} \overset{\text{iid}}{\sim} \mathbb{P}^*}\left[\mathbb{E}_{\mathbb{P}\sim\hat{\nu}}\left[\text{MMD}\left(\tilde{\mathbb{P}}, \mathbb{P}_{\theta^*(\mathbb{P})}\right)\right]\right]$$

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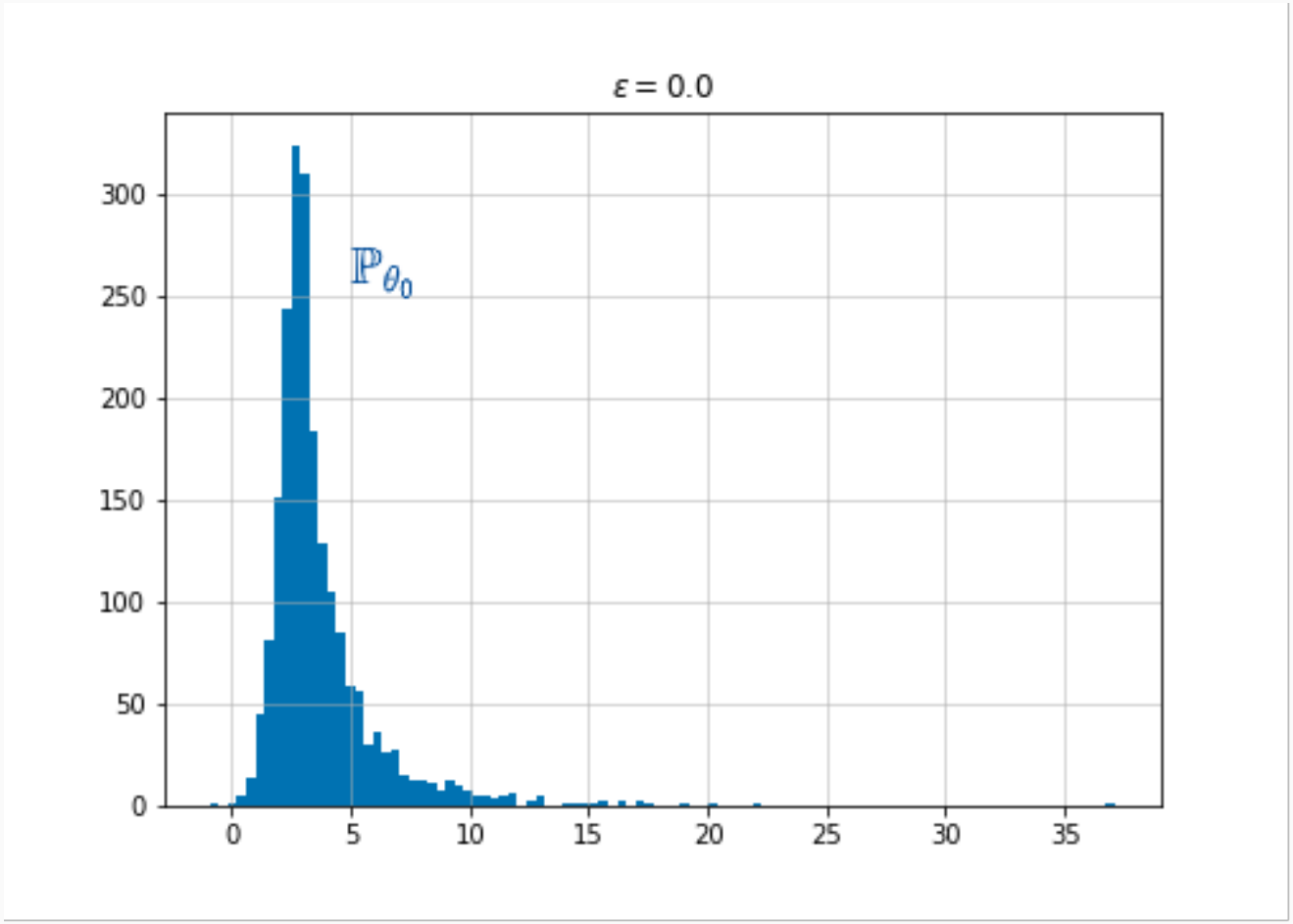
Applications

Example: Contaminated G-and-k distribution model

$\mathbb{P}^* = (1-\epsilon)\,\mathbb{P}_{\theta_0} + \epsilon\,\mathbb{Q}$ where $\mathbb{P}_{\theta_0}$ denotes the G-and-k distribution with $\theta_0 = (3, 1, 1, -\log(2))$, and $\mathbb{Q}$ is the shifted distribution $\mathbb{Q} = \mathbb{P}_{\theta_0} \pm 50$



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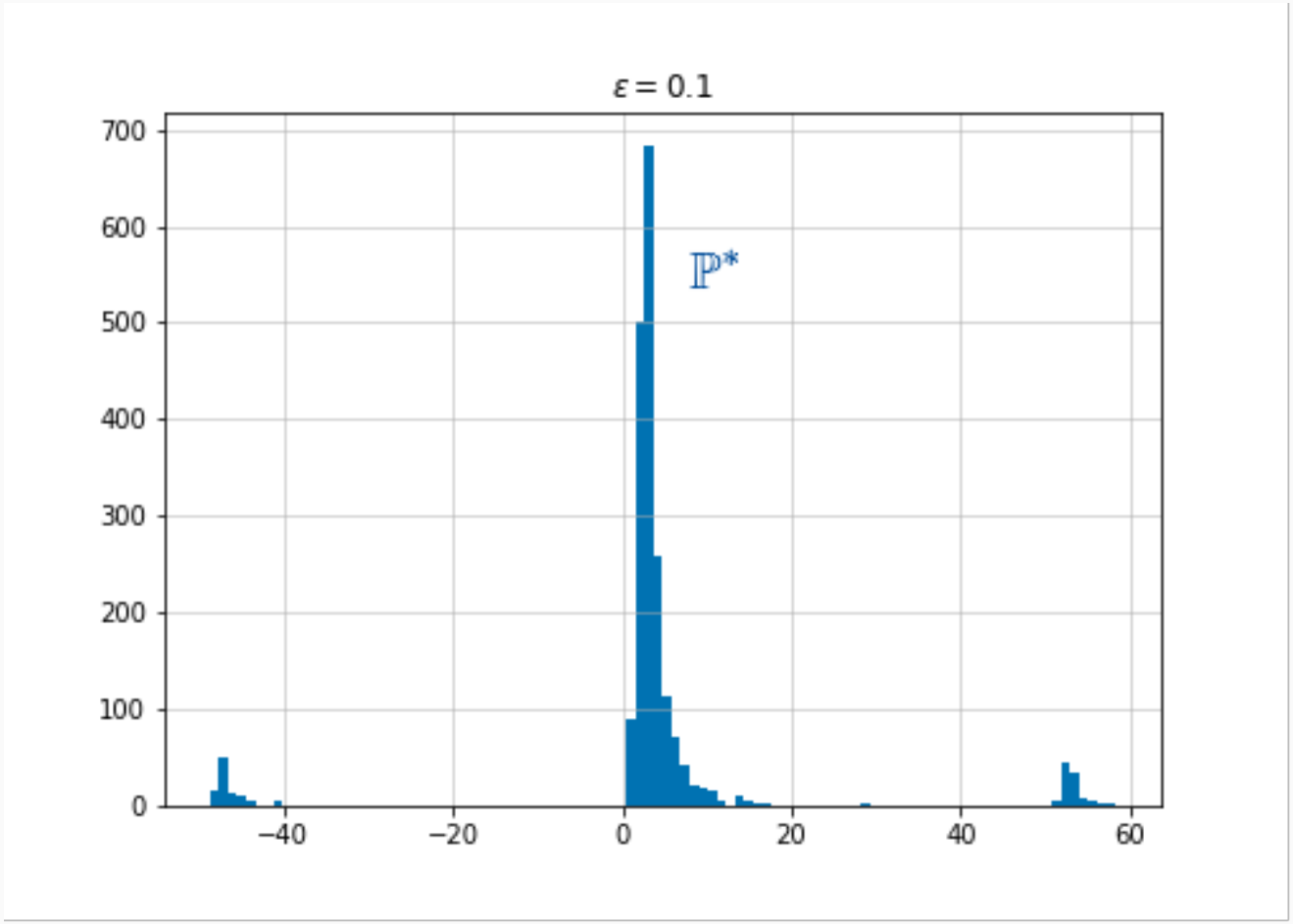

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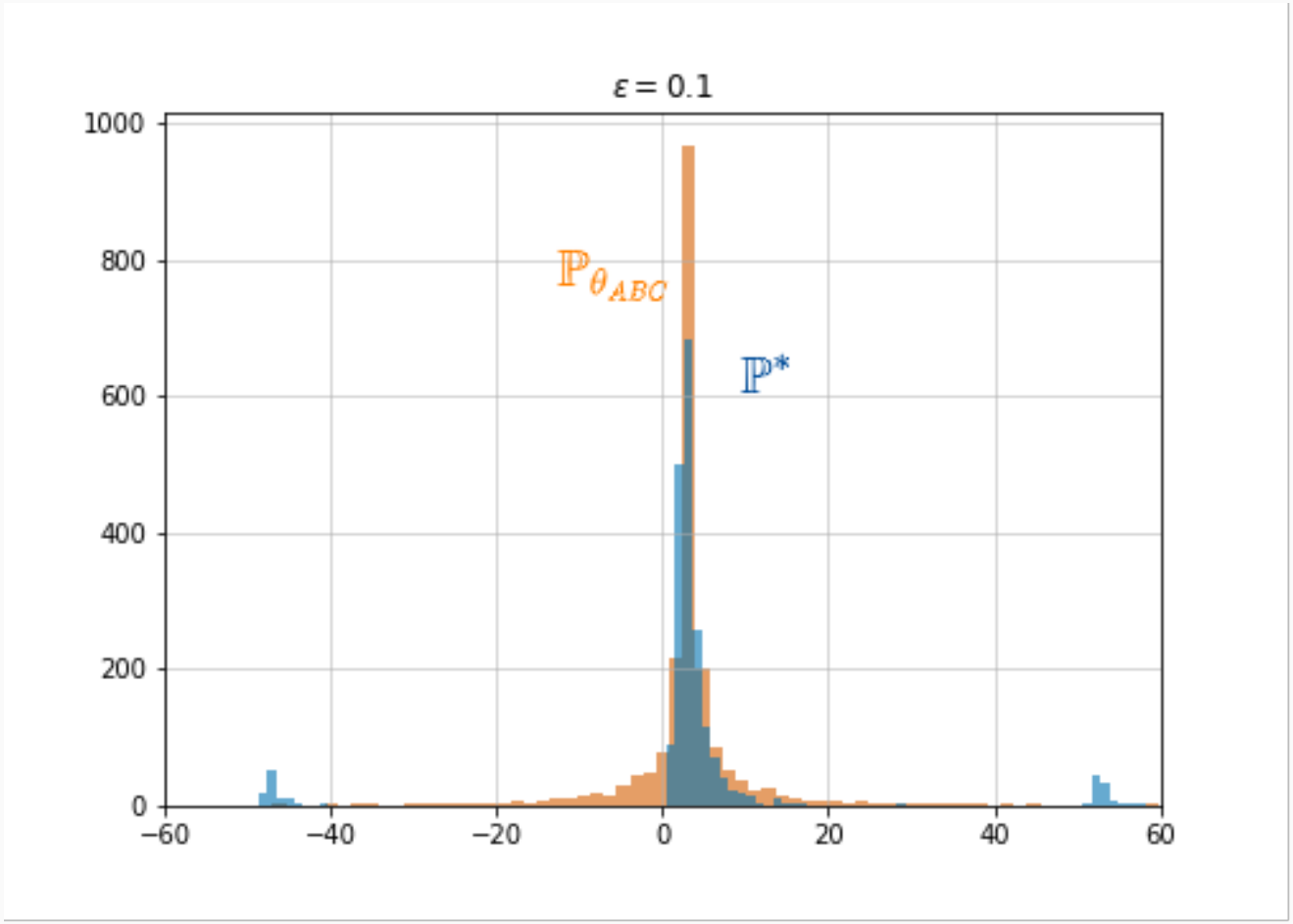

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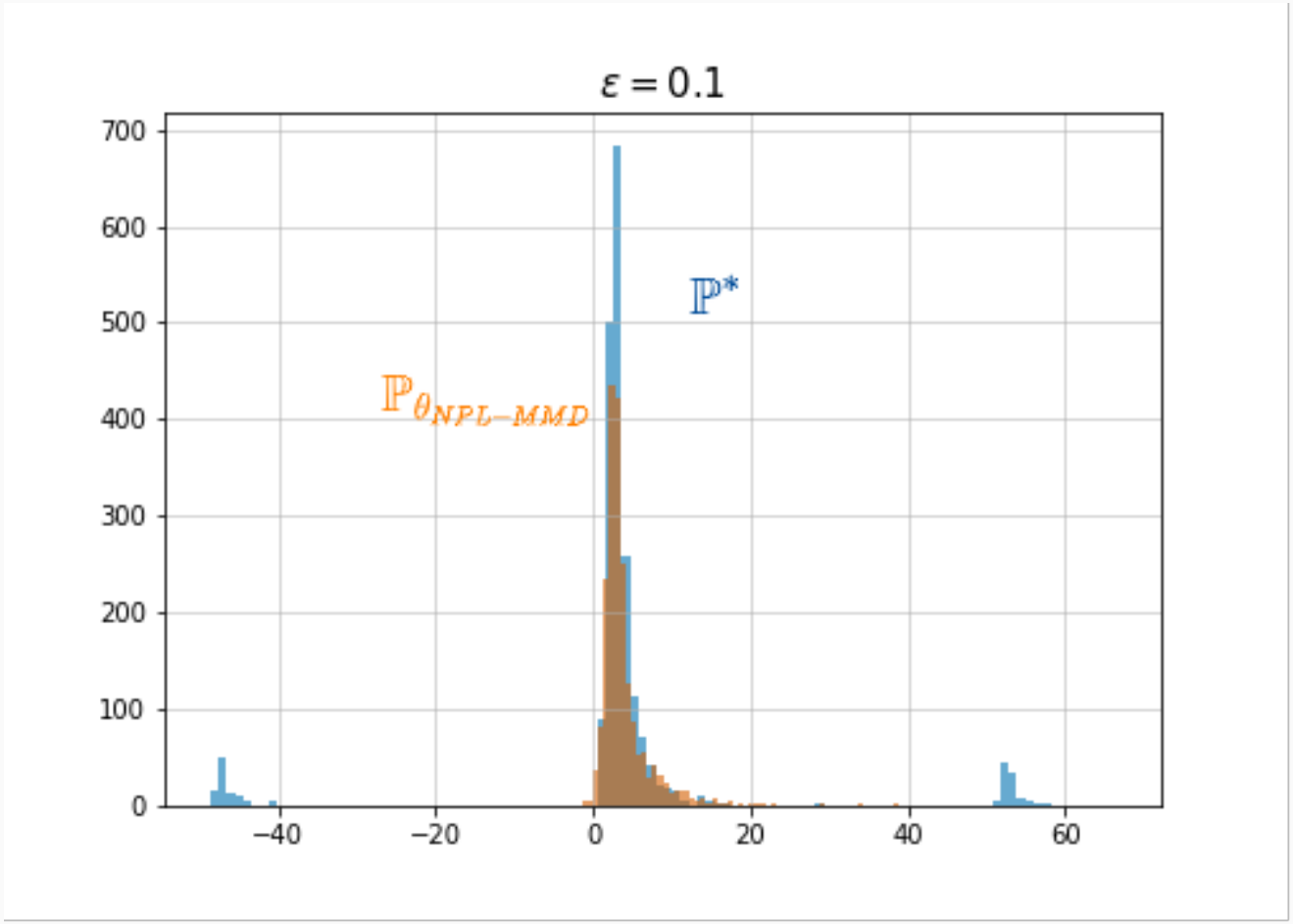

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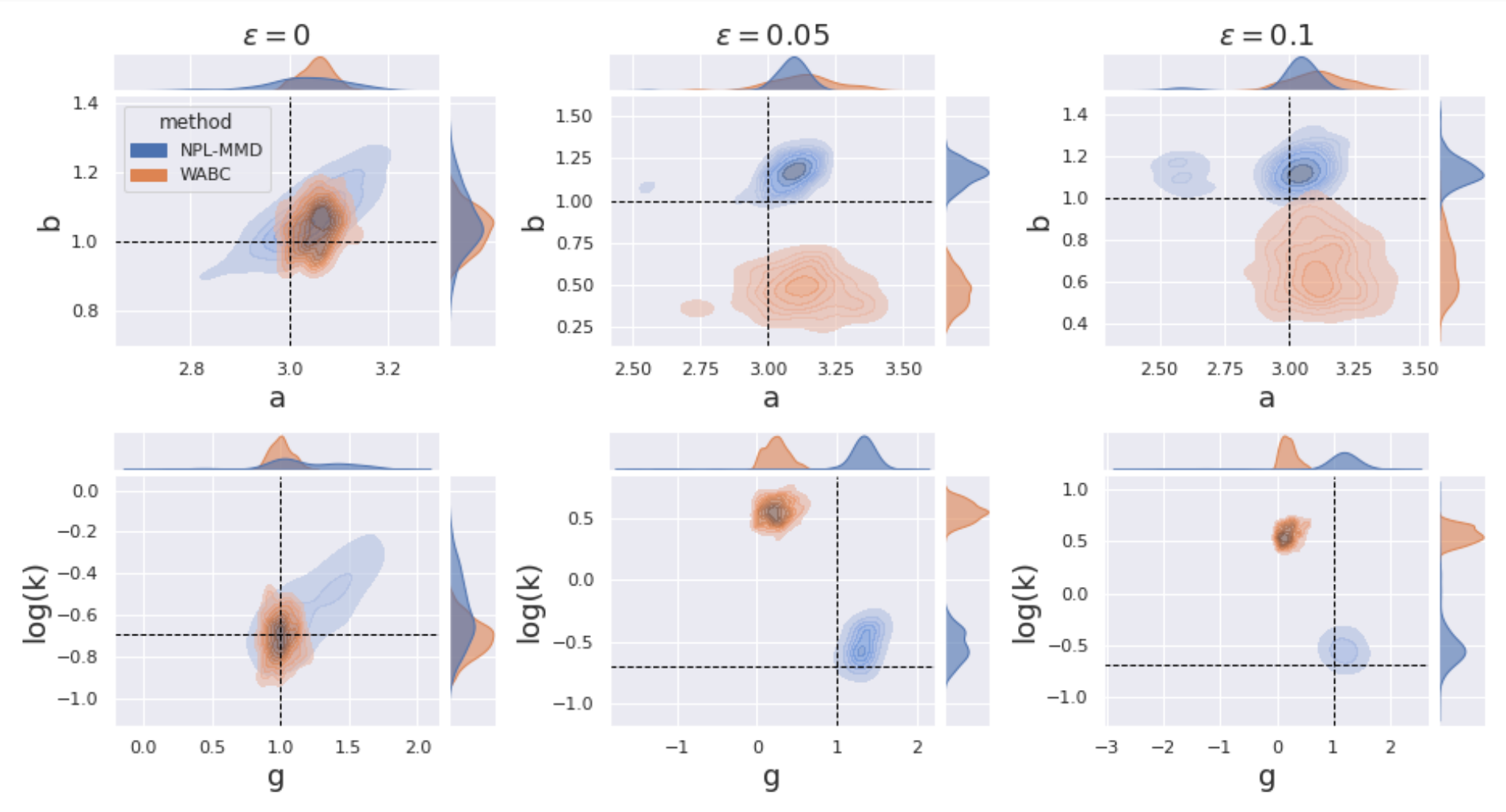

Figure 1: Comparison of posterior marginal distributions obtained using the MMD Posterior Bootstrap (NPL-MMD) and the Wasserstein-ABC (WABC) method in Bernton et al. (2019).

Example: Toggle switch model with Cauchy noise

- Arising in Systems Biology (see e.g. Bonassi et al., 2011)
- A dynamic model used to study cellular networks describing the interaction of two genes over time
- For cell i and unknown parameters $\theta = (\alpha_1, \alpha_2, \beta_1, \beta_2, \mu, \sigma, \gamma)^\top$, the simulator input is $u_i = (u_{i,1,1}, u_{i,1,2}, \ldots, u_{i,T,1}, u_{i,T,2}, u_{i,T+1,1})^\top \sim \text{Unif}([0,1]^{2T+1})$ and the simulator G_θ is defined through:

$$G_\theta(u_i) = \Phi^{-1}\left(\Phi\left(\frac{-(\mu+v_{i,T})v_{i,T}^{\gamma}}{\mu\sigma}\right) + u_{i,T+1,1}\left(1-\Phi\left(\frac{-(\mu+v_{i,T})v_{i,T}^{\gamma}}{\mu\sigma}\right)\right)\right)\frac{\mu\sigma}{v_{i,T}^{\gamma}} + (\mu + v_{i,T})$$

where for $t = 1, \ldots, T-1$, we have

$$\tilde{v}_{i,t+1} = v_{i,t} + \frac{\alpha_1}{1+w_{i,t}^{\beta_1}} - (1 + 0.03 v_{i,t})$$

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\end{aligned}$$

Example: Toggle switch model with Cauchy noise

- Inference on $\theta = (\alpha_1, \alpha_2, \beta_1, \beta_2, \mu, \sigma, \gamma)$ for $n = 2000$ data points simulated from the toggle-switch model in which 10% of the data have some added Cauchy noise of location parameter 0 and scale parameter 10.

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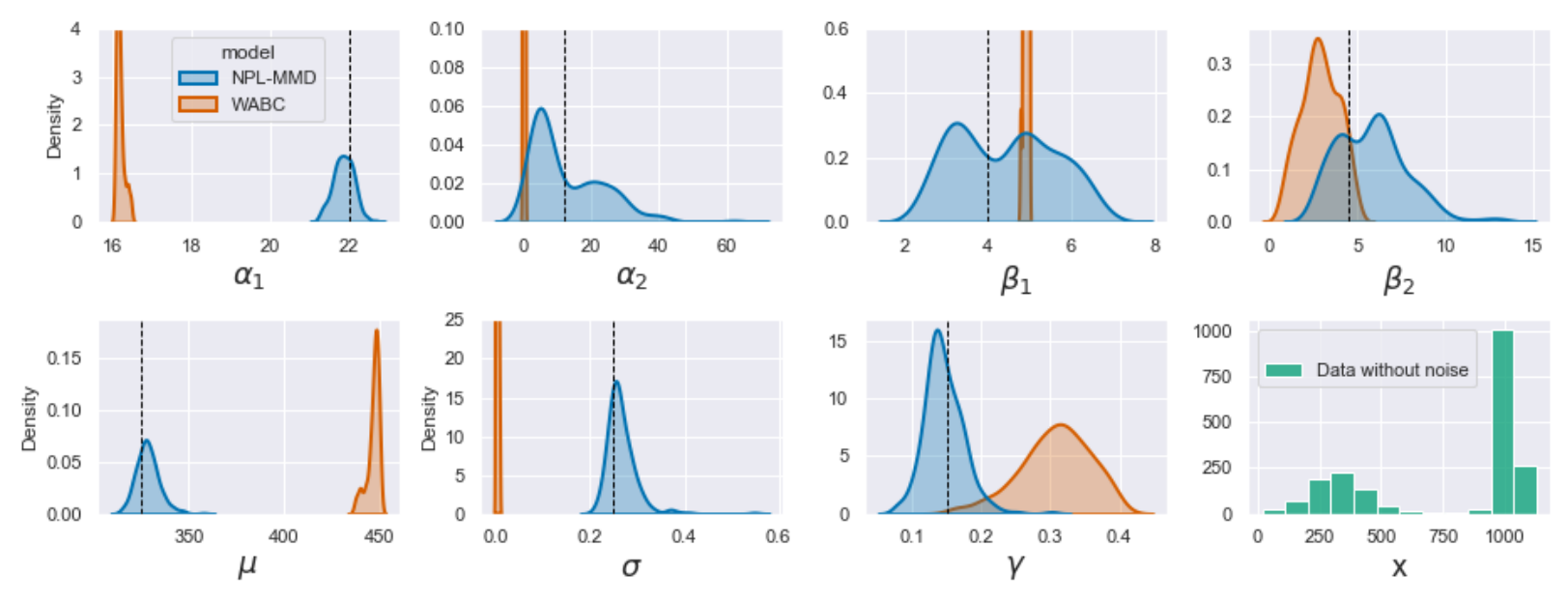

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