

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

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Outline

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 - Simulator-based models
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Motivation

Simulator-based models

- Independent sampling is possible, but the **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.



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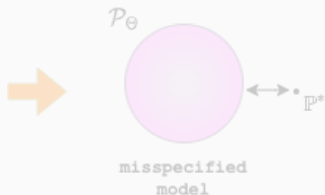
Simulator-based model family

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

\mathbb{P}_θ is associated with *simulator* function $G_\theta : \mathcal{U} \rightarrow \mathcal{X}$ 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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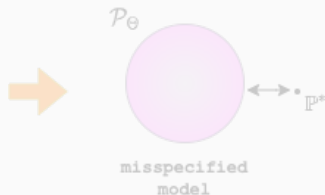
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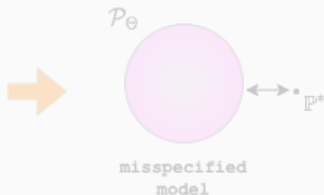
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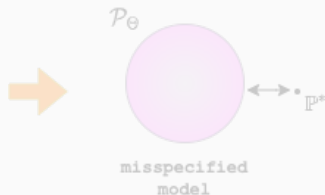
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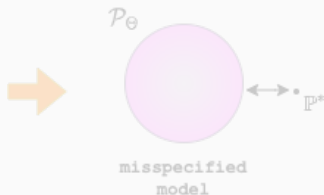
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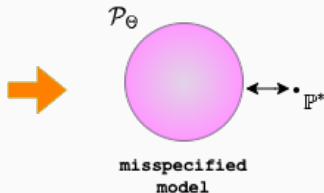
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- Bayesian inference via uncertainty coming from the data generating distribution while preserving robustness
 - ① **Approximate Bayesian Computation (ABC)** for ex. Bernton et al. (2019)
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Background

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

- Place a nonparametric prior *directly* on the data-generating mechanism \mathbb{P}^* :

$$\mathbb{P} \sim DP(\alpha, \mathbb{F}), \quad \mathbb{P}|_{\mathcal{X}_{1:n}} \sim DP(\alpha', \mathbb{F}')$$

where

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

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

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Push-forward measure

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

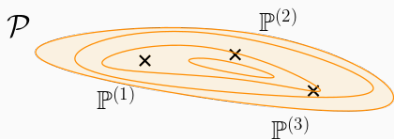
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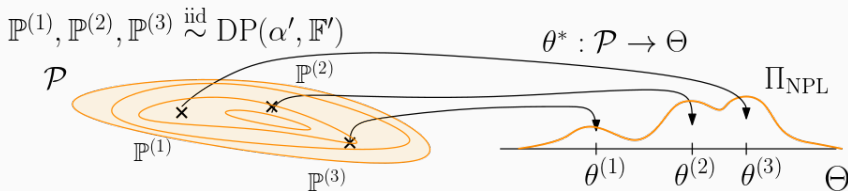
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Method

Distance-based loss function

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

- 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 $D : \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{R}_+$
- Minimisation of expected loss \longrightarrow Minimum Distance Estimation (MDE), Parr and Schucany (1980)

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- **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 $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, with associated norm $\|\cdot\|_{\mathcal{H}_k}$ and inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_k} : \mathcal{H}_k \times \mathcal{H}_k \rightarrow \mathbb{R}$.
- Reproducing property:
$$f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}_k}$$
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- 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):

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

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

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

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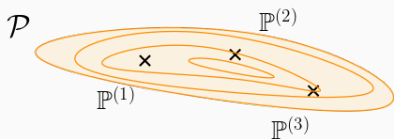
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MMD Posterior Bootstrap

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



• Draw $\mathbb{P}^{(j)} \sim DP(\alpha', \mathbb{F}')$

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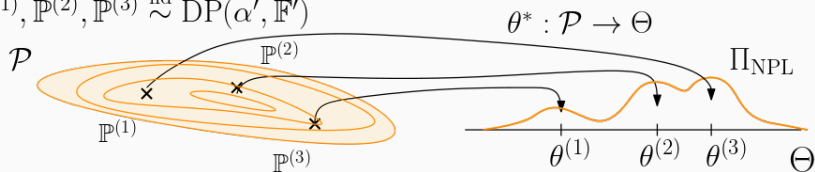
$$\tilde{x}_{1:T}^{(j)} \stackrel{\text{iid}}{\sim} \mathbb{F}, \quad (w_{1:n}^{(j)}, \tilde{w}_{1:T}^{(j)}) \sim \text{Dir}\left(1, \dots, 1, \frac{\alpha}{T}, \dots, \frac{\alpha}{T}\right).$$

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

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

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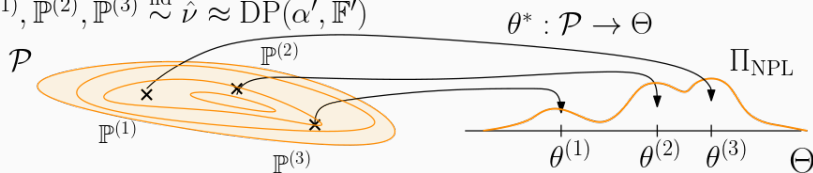
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Posterior Bootstrap with the MMD

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 $\tilde{x}_{1:T}^{(j)} \stackrel{\text{iid}}{\sim} \mathbb{F}$ and

$(w_{1:n}^{(j)}, \tilde{w}_{1:T}^{(j)}) \sim \text{Dir}(1, \dots, 1, \frac{\alpha}{T}, \dots, \frac{\alpha}{T})$.

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

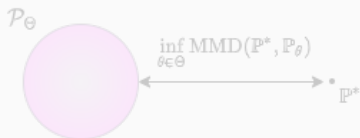
Obtain $\theta^{(j)} = \theta^*(\mathbb{P}^{(j)})$ using numerical optimisation.

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

Theoretical Results

Generalisation error

- **Assumption:** $\sup_{x, x' \in \mathcal{X}} |k(x, x')| < \infty$
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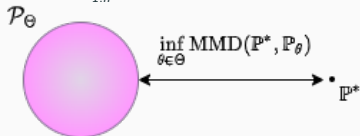
$$\mathbb{E}_{x_{1:n} \stackrel{\text{iid}}{\sim} \mathbb{P}^*} [\mathbb{E}_{\mathbb{P} \sim \nu} [\text{MMD}(\mathbb{P}^*, \mathbb{P}_{\theta^*(\mathbb{P})})]]$$

\mathcal{P}_θ \longleftrightarrow \mathbb{P}^*
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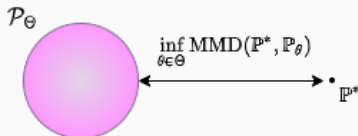
$$\inf_{\theta \in \Theta} \text{MMD}(\mathbb{P}^*, \mathbb{P}_\theta) \leq \mathbb{E}_{x_{1:n} \stackrel{\text{iid}}{\sim} \mathbb{P}^*} [\mathbb{E}_{\mathbb{P} \sim \nu} [\text{MMD}(\mathbb{P}^*, \mathbb{P}_{\theta^*(\mathbb{P})})]]$$



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$$\begin{aligned} 0 &\leq \overbrace{\mathbb{E}_{x_{1:n} \stackrel{\text{iid}}{\sim} \mathbb{P}^*} [\mathbb{E}_{\mathbb{P} \sim \nu} [\text{MMD}(\mathbb{P}^*, \mathbb{P}_{\theta^*(\mathbb{P})})]] - \inf_{\theta \in \Theta} \text{MMD}(\mathbb{P}^*, \mathbb{P}_\theta)}^{\text{Generalisation Error}} \\ &\leq \frac{2}{\sqrt{n}} + \frac{2}{\sqrt{\alpha + n + 2}} + \frac{4\alpha}{\alpha + n} \end{aligned}$$



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

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

$$\Pi_n \left(\theta \in \Theta : \text{MMD}(\mathbb{P}_\theta, \mathbb{P}^*) > \inf_{\theta \in \Theta} \text{MMD}(\mathbb{P}_\theta, \mathbb{P}^*) + \frac{M_n}{n^{1/2}} \right) \xrightarrow{n \rightarrow \infty} 0 \quad (2)$$

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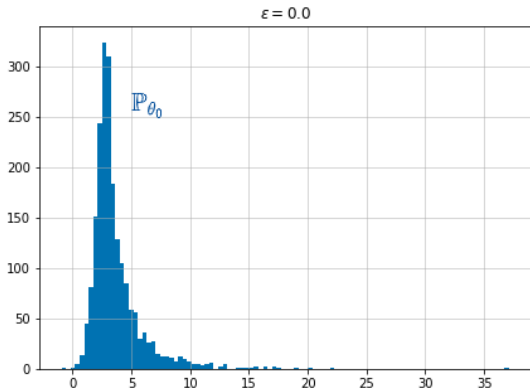
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Applications

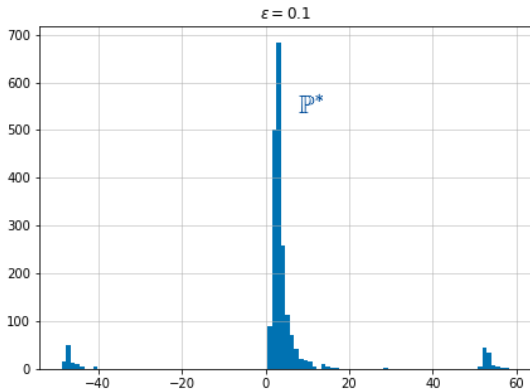
Example: Contaminated G-and-k distribution model

$\mathbb{P}^* = (1 - \epsilon)\mathbb{P}_{\theta_0} + \epsilon\mathbb{Q}$ where \mathbb{P}_{θ_0} denotes the G-and-k distribution with $\theta_0 = (3, 1, 1, -\log(2))$, and \mathbb{Q} is the shifted distribution $\mathbb{Q} = \mathbb{P}_{\theta_0} \pm 50$



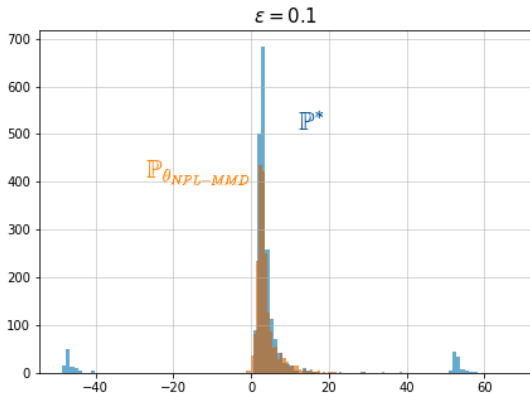
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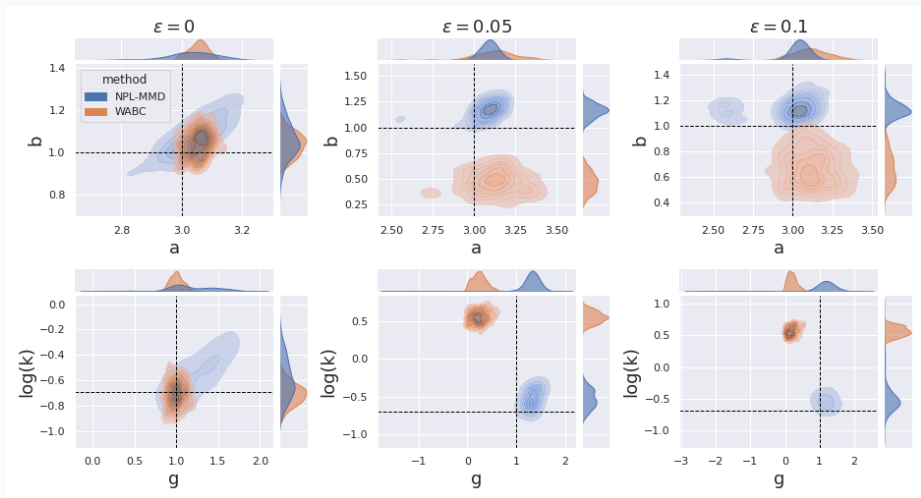


Figure 1: Comparison of posterior marginal distributions obtained using the MMD Posterior Bootstrap (NPL-MMD) and the Wasserstein-ABC (WABC) method in Bernton et al. (2019).

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 $u_i = (u_{i,1,1}, u_{i,1,2}, \dots, u_{i,T,1}, u_{i,T,2}, u_{i,T+1,1})^\top \sim \text{Unif}([0, 1]^{2T+1})$ 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 $t = 1, \dots, T - 1$, we have

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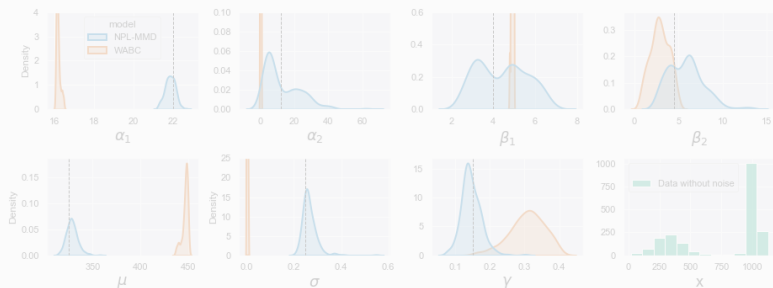
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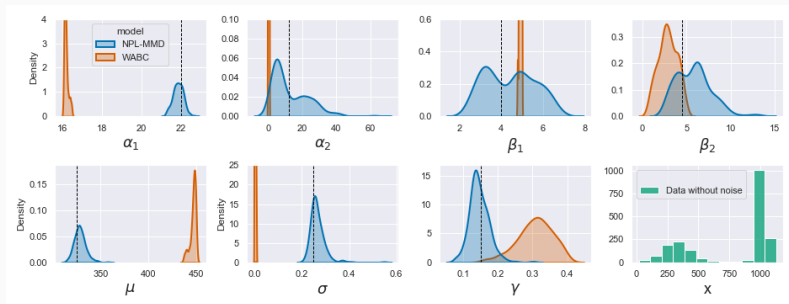
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Discussion & current work

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- ✓ Posterior Bootstrap algorithm suitable for simulator-based models inducing robustness through:
 - Bayesian Nonparametric Learning (NPL) framework
 - Minimum Maximum Mean Discrepancy (MMD) estimators
- ✓ Highly parallelisable algorithm
- ✓ Generalisation error, posterior consistency and robustness to outliers guarantees

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- Covariate X is only observed via a *noisy* proxy W such that:

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Goal: to estimate θ_0 when data from (W, Y) is available

- We do **not** have observations from \mathbb{P}^* anymore!
- If our model assumes that there is no ME, how can we be robust?
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