Learning Robust Statistics for Simulation-based Inference under Model Misspecification

Daolang Huang*[1], Ayush Bharti*[1], Amauri Souza[1], Luigi Acerbi[2], Samuel Kaski[1,3]

Department of Computer Science, Aalto University[1]
Department of Computer Science, University of Helsinki[2]
Department of Computer Science, University of Manchester[3]

December 1, 2023

Simulation-based inference

- Data $\mathbf{y} = \{y_i\}_{i=1}^n \subseteq \mathbb{R}^d$ denoted by empirical distribution $\mathbb{Q}^n$
- Simulator-based model $\mathcal{P}_\Theta = \{\mathbb{P}_\theta : \theta \in \Theta\}$
- $\mathbb{P}_\theta$ is intractable, but sampling $\mathbf{x} \sim \mathbb{P}_\theta$ is straightforward
- **Aim:** Estimate θ given data $\mathbf{y}$

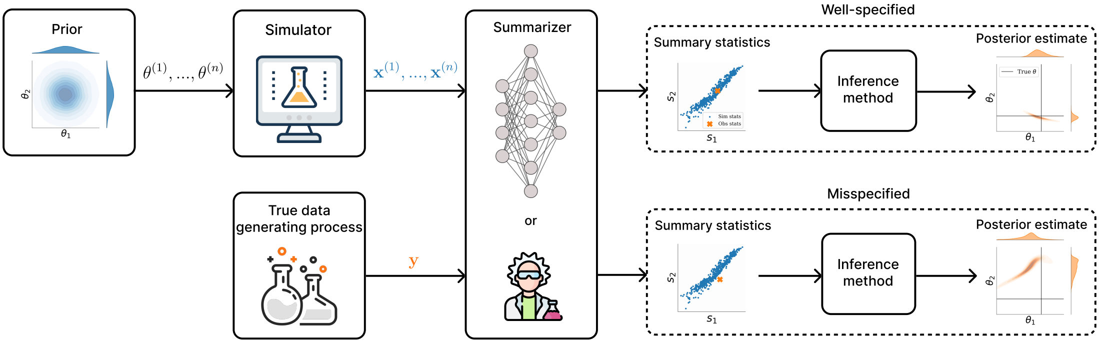
Simulation-based inference

- Data $\mathbf{y} = \{y_i\}_{i=1}^n \subseteq \mathbb{R}^d$ denoted by empirical distribution $\mathbb{Q}^n$
- Simulator-based model $\mathcal{P}_\Theta = \{\mathbb{P}_\theta : \theta \in \Theta\}$
- $\mathbb{P}_\theta$ is intractable, but sampling $\mathbf{x} \sim \mathbb{P}_\theta$ is straightforward
- **Aim:** Estimate θ given data $\mathbf{y}$
- **Solution:** methods based on distances like approximate Bayesian computation (ABC); methods based on deep neural networks like neural posterior estimation (NPE)

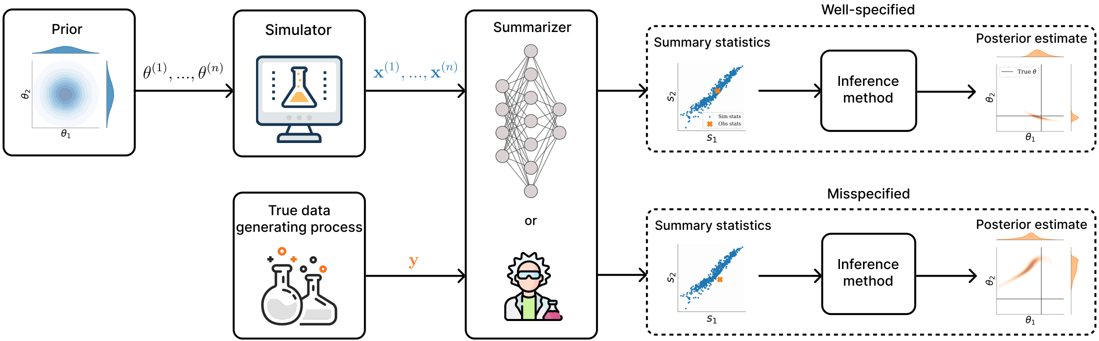
Simulation-based inference

- Data $\mathbf{y} = \{y_i\}_{i=1}^{n} \subseteq \mathbb{R}^d$ denoted by empirical distribution $\mathbb{Q}^n$
- Simulator-based model $\mathcal{P}_\Theta = \{\mathbb{P}_\theta : \theta \in \Theta\}$
- $\mathbb{P}_\theta$ is intractable, but sampling $\mathbf{x} \sim \mathbb{P}_\theta$ is straightforward
- **Aim:** Estimate θ given data $\mathbf{y}$
- **Assumption:** Model is "correct", i.e., $\mathbb{Q}^n \in \mathcal{P}_\Theta$
- **Problem:** Model misspecification, i.e. $\mathbb{Q}^n \notin \mathcal{P}_\Theta \Rightarrow \nexists \theta \in \Theta$ s.t. $\mathbb{P}_\theta = \mathbb{Q}^n$
  - Stochasticity in data collection process (outliers, missing data, broken independence assumption, etc.)
  - "All models are wrong..."
- **Even more problem:** Inference is based on simulation from misspecified model!

Inference is based on summary statistics



Inference is based on summary statistics



Insight 1: Under misspecification, observed statistic goes outside the set of simulated statistics

$\Rightarrow$ SBI methods have to generalize outside their training data

Insights

Insight 1: Under misspecification, observed statistic goes outside the set of simulated statistics

$\Rightarrow$ SBI methods have to generalize outside their training data

Insight 2: Even if model is misspecified ($\mathbb{Q}^n \notin \mathcal{P}_\Theta$), it may be well-specified w.r.t the statistics

- Example: Gaussian model, skewed data
- Misspecified if statistics are sample mean and sample skewness
- Well-specified if statistics are sample mean and sample variance
- If we pick statistics appropriately, we can be robust!

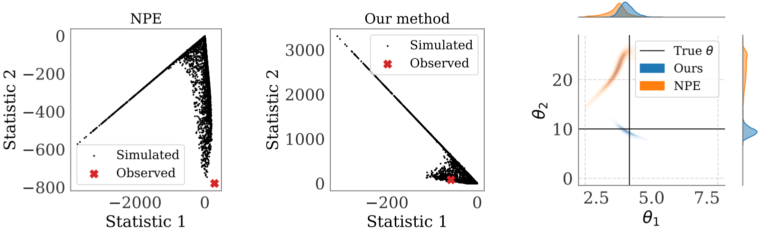
Learning robust statistics for SBI

proposed loss $=$ usual loss $+$ $\lambda\mathcal{D}$(simulated statistics, observed statistic)

Learning robust statistics for SBI

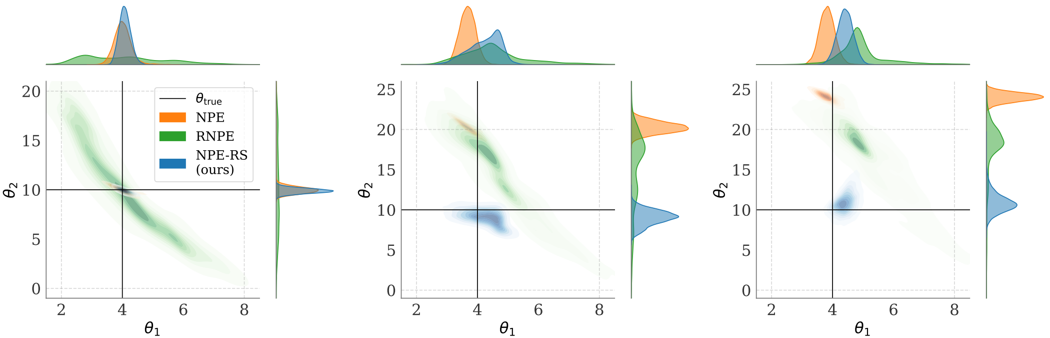
$$\text{proposed loss} = \text{usual loss} + \lambda\mathcal{D}(\text{simulated statistics, observed statistic})$$

- For ABC or other SBI methods, usual loss is autoencoder's reconstruction loss
- For NPE, statistics and posterior can be learned jointly
- We want $\mathcal{D}$ to be outlier-robust. Hence, maximum mean discrepancy.
- Regularizer λ: encodes trade-off between accuracy and robustness



Results

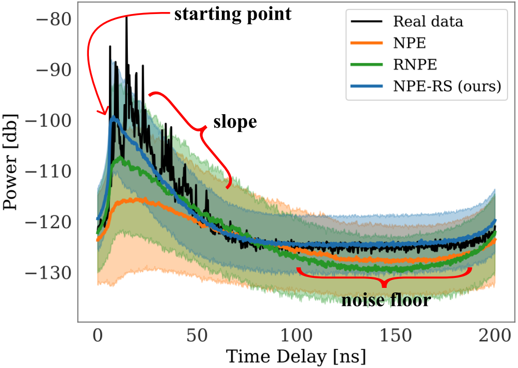
- **Ricker model:** 2 parameters
- **Inference method:** Neural posterior estimation (NPE)
- **ϵ-contamination model:** $\mathbb{Q} = (1-\epsilon)\mathbb{P}_{\theta_{\text{true}}} + \epsilon\mathbb{P}_{\theta_c}$



(a) Well-specified ($\epsilon = 0$) (b) Misspecified ($\epsilon = 10\%$) (c) Misspecified ($\epsilon = 20\%$)

Radio propagation example

- 4 parameters
- Data dimension: 801
- Model misspecified due to broken iid assumption



Conclusion

- We propose a simple solution for tackling misspecification of simulator-based models.
- Our method can be applied to any SBI method that utilizes summary statistics.
- Our method only has one hyperparameter balancing efficiency and robustness.
- We show robustness under misspecified scenarios with both synthetic and real-world data.