Leveraging Self-Consistency for Data-Efficient Amortized Bayesian Inference

NeurIPS 2023, UniReps workshop











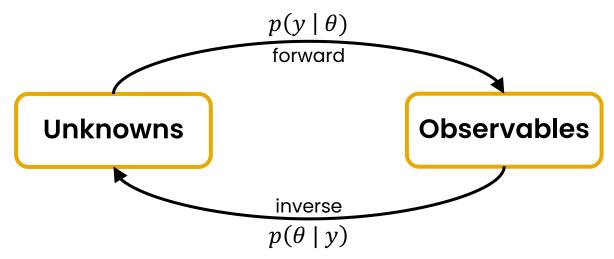
Marvin Schmitt

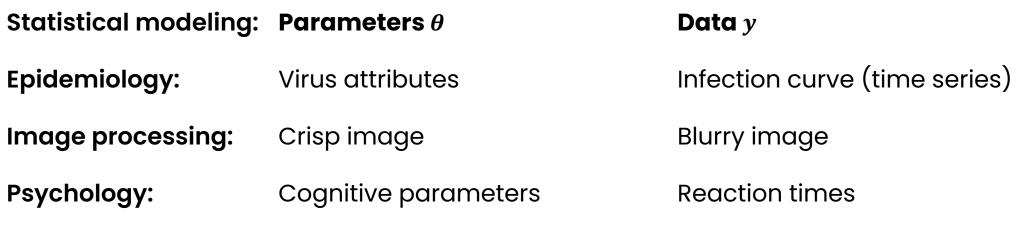
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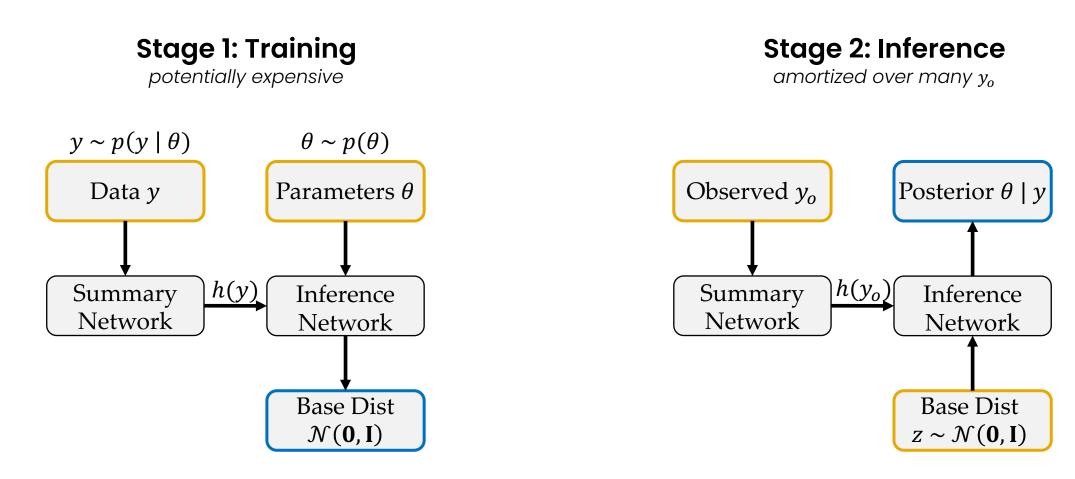
Stefan Radev

Inverse Problems





Amortized Bayesian Inference



Self-Consistency Property

 \times

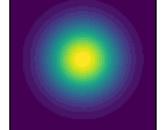
$$p(y) = p(\theta) p(y | \theta) / p(\theta | y) \implies \frac{p(\tilde{\theta}_1) p(y | \tilde{\theta}_1)}{p(\tilde{\theta}_1 | y)} = \dots = \frac{p(\tilde{\theta}_K) p(y | \tilde{\theta}_K)}{p(\tilde{\theta}_K | y)} \quad \tilde{\theta}_1, \dots, \tilde{\theta}_K \in \Theta$$

Symmetry

Approximation

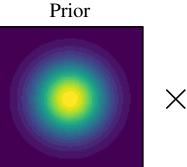
Posterior

Perfect



Prior



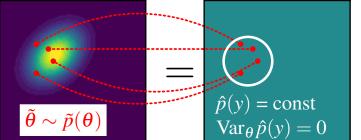




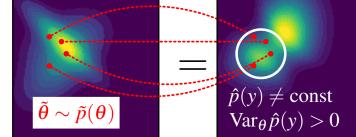
Likelihood

True posterior





Approximate posterior Est. marginal likelihood



Self-Consistency Loss

• Idea: Violations of self-consistency property as loss function

$$\mathcal{L}_{\mathrm{SC}} := \mathbb{E}_{p(y)} \Big[\operatorname{Var}_{\tilde{\theta} \sim \tilde{p}(\theta)} \Big(\log p(\tilde{\theta}) + \log p(y \,|\, \tilde{\theta}) - \log q_{\phi}(\tilde{\theta} \,|\, y) \Big) \Big]$$

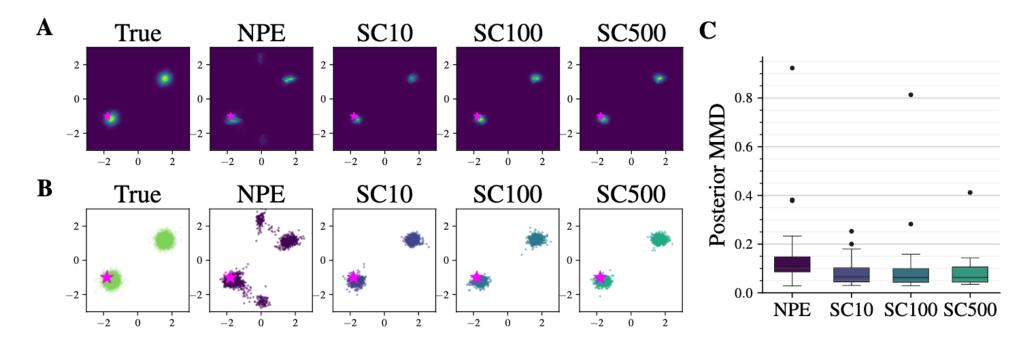
• Integration into standard neural posterior estimation loss

$$\mathcal{L}_{\text{NPE-SC}} := \mathbb{E}_{p(y)} \Big[\underbrace{\mathbb{E}_{p(\theta \mid y)} \Big[-\log q_{\phi}(\theta \mid y) \Big]}_{\text{NPE loss}} + \underbrace{\lambda \operatorname{Var}_{\tilde{\theta} \sim \tilde{p}(\theta)} \left(\log p(\tilde{\theta}) + \log p(y \mid \tilde{\theta}) - \log q_{\phi}(\tilde{\theta} \mid y) \right)}_{\text{self-consistency loss } \mathcal{L}_{\text{SC}} \text{ with weight } \lambda \in \mathbb{R}_{+}} \Big]$$

Experiment 1: Gaussian Mixture

Posterior estimation, N = 1024 training budget

- Model: $\theta \sim \mathcal{N}(\theta \,|\, \mathbf{0}, \mathbf{I}), \qquad y \sim 0.5 \, \mathcal{N}(y \,|\, \theta, \mathbf{I}/2) + 0.5 \, \mathcal{N}(y \,|\, -\theta, \mathbf{I}/2)$
- **Results**: Better density and sampling compared to default (NPE)

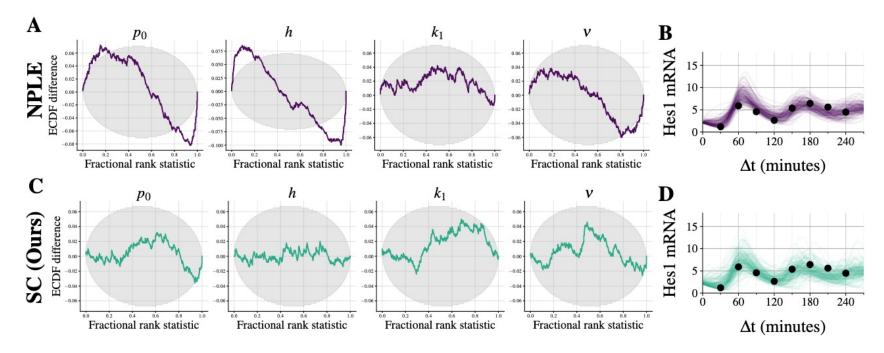


Experiment 2: Hes1 Expression Model

Posterior and likelihood estimation, N = 512 training budget

Results:

- Better simulation-based calibration (SBC; Talts et al., 2018)
- Similar posterior predictive results



Conclusion & Next Steps

Achievements

- Better posterior estimation in low-data settings
- Straightforward integration of the additive self-consistency loss

Next steps

- Explore better and more stable self-consistency training schemes
- Push the envelope on training/inference without ground-truths
- Potential for out-of-distribution settings?

Contact











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