

Neural posterior estimation

Likelihood-free inference

Train a *conditional* neural network w/ *in silico* simulations on pairs $\{(\mathbf{x}^{(m)}, \mathbf{y}^{(m)})\}_{m=1}^M$

$$\mathbf{y} \sim p(\mathbf{y} | \mathbf{x}) \quad \Longleftrightarrow \quad \mathbf{y} = \mathbf{g}(\mathbf{x}, \boldsymbol{\zeta})$$

$$\text{where } \boldsymbol{\zeta} \sim p(\boldsymbol{\zeta} | \mathbf{x}) \quad \text{with } \mathbf{x} \sim p(\mathbf{x})$$

Given these pairs train via

$$\underset{\phi, \psi}{\text{minimize}} \frac{1}{M} \sum_{m=1}^M \left(\frac{1}{2} \left\| f_{\phi} \left(\mathbf{x}^{(m)}; h_{\psi}(\mathbf{y}^{(m)}) \right) \right\|_2^2 - \log \left| \det J_{f_{\phi}}^{(m)} \right| \right)$$

► f_{ϕ} is the *inference network* defined by a *Conditional Normalizing Flow* (CNF)

► h_{ψ} is a learned *summary* statistic yielding $MI \left(\mathbf{x}, h_{\psi}(\mathbf{y}) \right) \approx MI \left(\mathbf{x}, \mathbf{y} \right)$

Summary statistic

physics-based

Assume Gaussian log-likelihood:

$$\log p(\mathbf{y} | \mathbf{x}) = -\frac{1}{2} \|\mathcal{H}(\mathbf{x}) - \mathbf{y}\|_2^2$$

Use score function at *fiducial* point $\bar{\mathbf{x}}$:

$$p(\mathbf{x} | \nabla_{\mathbf{x}} \log p(\mathbf{y} | \mathbf{x}) \Big|_{\bar{\mathbf{x}}}) \approx p(\mathbf{x} | \mathbf{y})$$

in combination w/ learned *summary network* yields

$$\bar{\mathbf{y}} = h_{\psi}(\mathbf{J}_{\mathcal{H}}^{\top}(\bar{\mathbf{x}})(\mathcal{H}(\bar{\mathbf{x}}) - \mathbf{y}))$$

such that

$$p(\mathbf{x} | \bar{\mathbf{y}}) \approx p(\mathbf{x} | \mathbf{y})$$