

Neural posterior estimation

Likelihood-free inference

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

$$\mathbf{y} \sim p(\mathbf{y} \mid \mathbf{x}) \iff \mathbf{y} = \mathbf{g}(\mathbf{x}, \boldsymbol{\zeta})$$
where $\boldsymbol{\zeta} \sim p(\boldsymbol{\zeta} \mid \mathbf{x})$ with $\mathbf{x} \sim p(\mathbf{x})$

Given these pairs train via

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

- $ightharpoonup f_{\phi}$ is the *inference network* defined by a Conditional Normalizing Flow (CNF)
- $\blacktriangleright h_{\psi}$ is a learned *summary* statistic yielding $MI\left(\mathbf{x},h_{\psi}(\mathbf{y})\right)pprox MI\left(\mathbf{x},\mathbf{y}\right)$

SLIM (4)
ML4Seismic

Orozco, Rafael, et al. "Adjoint operators enable fast and amortized machine learning based Bayesian uncertainty quantification." Medical Imaging 2023: Image Processing. Vol. 12464. SPIE, 2023.

Alsing, Justin, Benjamin Wandelt, and Stephen Feeney. "Massive optimal data compression and density estimation for scalable, likelihood-free inference in cosmology." Monthly Notices of the Royal Astronomical Society 477.3 (2018): 2874-2885.

Summary statistic physics-based

Assume Gaussian log-likelihood:

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

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

$$p(\mathbf{x} \mid \nabla_{\mathbf{x}} \log p(\mathbf{y} \mid \mathbf{x}) \mid_{\bar{\mathbf{x}}}) \approx p(\mathbf{x} \mid \mathbf{y})$$

in combination w/ learned summary network yields

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

such that

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