Simulation-Based Inference

February 15, 2022

Algorithm 1: Training Procedure.

Input: Forward model f, prior over physical parameters $\mathrm{P}(\mathbf{z})$.
Output: Approximate posterior $\mathrm{Q}_\phi(\mathbf{z}|\mathbf{x})$. Also a likelihood $\mathrm{P}_{\mathbf{W}}(\mathbf{x}|\mathbf{z})$.

repeat

  Simulate $\{(\mathbf{z}_i, \mathbf{x}_i)\}_{i=1}^N$ pairs, using $\mathbf{x}_i \leftarrow f(\mathbf{z}_i)$, $\mathbf{z}_i \sim \mathrm{P}(\mathbf{z}_i)$.

  Train $\mathrm{Q}_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ via ML:

$$\arg\max_{\boldsymbol{\phi}} \sum_{i=1}^{N} \log \mathrm{Q}_{\boldsymbol{\phi}}(\mathbf{z}_i|\mathbf{x}_i)$$

  Train a neural likelihood (or likelihood-ratio?)

$$\arg\max_{\mathbf{W}} \sum_{i=1}^{N} \log \mathrm{P}_{\mathbf{w}}(\mathbf{x}_i|\mathbf{z}_i)$$

  Minimise a divergence (e.g. D_{KL}):

$$\arg\min_{\boldsymbol{\phi}} D_{\mathrm{KL}}\big[\mathrm{Q}_\phi(\mathbf{z}|\mathbf{x}_{\mathrm{true}}) \| \mathrm{P}(\mathbf{z}|\mathbf{x}_{\mathrm{true}})\big]$$

  where $\mathrm{P}(\mathbf{z}|\mathbf{x}_{\mathrm{true}}) \propto \mathrm{P}_{\mathbf{W}}(\mathbf{x}_{\mathrm{true}}|\mathbf{z})\mathrm{P}(\mathbf{z})$.

until *Until reconstructions match the data*

The ELBO has the following form:

$$\mathcal{L}(\phi) = \mathbb{E}_{\mathrm{Q}_\phi(\mathbf{z}|\mathbf{x}_{\mathrm{true}})}\big[\log \mathrm{P}(\mathbf{z}, \mathbf{x}_{\mathrm{true}}) - \log \mathrm{Q}_\phi(\mathbf{z}|\mathbf{x}_{\mathrm{true}})\big] \quad (1)$$

$$= \mathbb{E}_{\mathrm{Q}_\phi(\mathbf{z}|\mathbf{x}_{\mathrm{true}})}\left[\log \mathrm{P}_{\mathbf{W}}(\mathbf{x}_{\mathrm{true}}|\mathbf{z}) - \log \frac{\mathrm{Q}_\phi(\mathbf{z}|\mathbf{x}_{\mathrm{true}})}{\mathrm{P}(\mathbf{z})}\right] \quad (2)$$

We optimise an MC approximation of this objective, using K terms

$$\mathcal{L}(\phi) \approx \sum_{i=1}^{K} \log \mathrm{P}_{\mathbf{W}}(\mathbf{x}_{\mathrm{true}:j}|\mathbf{z}_i) - \log \mathrm{Q}_\phi(\mathbf{z}_i|\mathbf{x}_{\mathrm{true}:j}) + \log \mathrm{P}(\mathbf{z}_i),$$

where $\mathbf{z}_i \sim \mathrm{Q}_\phi(\mathbf{z}_i|\mathbf{x}_{\mathrm{true}:j})$.