Simulation-Based Inference

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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}):

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

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*