

Relation

conditional neural density & EIG

Maximizing the expected *posterior density* is *equivalent* to maximizing the expected *information gain*

$$\begin{aligned}\max_{\mathbf{W}} \text{EIG}(\mathbf{W}) &= \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[D_{KL}(p_{\theta}(\mathbf{x}|\mathbf{y}) || p(\mathbf{x})) \right] = \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[\mathbb{E}_{p(\mathbf{x}|\mathbf{y})} \left[\log p_{\theta}(\mathbf{x}|\mathbf{y}) - \log p(\mathbf{x}) \right] \right] \\ &= \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[\mathbb{E}_{p(\mathbf{x}|\mathbf{y})} \left[\log p_{\theta}(\mathbf{x}|\mathbf{y}) \right] \right] \text{ law of total expectation} \\ &= \mathbb{E}_{p(\mathbf{x},\mathbf{y}|\mathbf{W})} \left[\log p_{\theta}(\mathbf{x}|\mathbf{y}) \right] \text{ same as neural posterior objective!}\end{aligned}$$

Thus optimizing under the posterior density objective will increase the EIG!

Proposed method

As usual, prepare posterior learning algorithm: $\{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{i=1}^N$

Instead of optimizing only network parameters:

$$\hat{\theta} = \arg \max_{\theta} \frac{1}{N} \sum_{n=1}^N \left(-\|f_{\theta}(\mathbf{x}^{(n)}; \bar{\mathbf{y}}^{(n)})\|_2^2 + \log \left| \det \mathbf{J}_{f_{\theta}} \right| \right).$$

Jointly optimize experimental design in terms of **density**, \mathbf{w} , defining the mask $\mathbf{M}(\mathbf{w})$

$$\hat{\theta}, \hat{\mathbf{w}} = \arg \max_{\theta, \mathbf{w}} \frac{1}{N} \sum_{i=1}^N \left(-\|f_{\theta}(\mathbf{x}^{(n)}; (\mathbf{W}[\mathbf{w}] \odot \mathbf{x}^{(n)}, \bar{\mathbf{y}}^{(n)}))\|_2^2 + \log \left| \det \mathbf{J}_{f_{\theta}} \right| \right).$$