Homework 6

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Lecture on BFNs and AI4Science

Question 1:

Suppose our goal is to estimate the unknown y given some observations x. Prove that the optimal solution $\hat{y}$ to the MSE loss $L(\hat{y}) = \mathbb{E}_{y\sim p(y|x)}[(y-\hat{y})^2]$ is the posterior expectation $\hat{y}^* = \mathbb{E}[y|x]$, and explain the role of $p(y|x)$ in the context of Bayesian inference.

Answer:

$$\begin{aligned}
\hat{y}^* &= \arg\min_{\hat{y}} \ \mathbb{E}_{y\sim p(y|x)}[(y-\hat{y})^2] \\
&= \arg\min_{\hat{y}} \ \mathbb{E}_{y\sim p(y|x)}[y^2 - 2y\hat{y} + \hat{y}^2] \\
&= \arg\min_{\hat{y}} \ \mathbb{E}_{y\sim p(y|x)}[y^2] - 2\hat{y}\ \mathbb{E}_{y\sim p(y|x)}[y] + \hat{y}^2
\end{aligned}$$

This quadratic function in $\hat{y}$ reaches its minimum at the vertex of the parabola, which gives $\hat{y}^* = \mathbb{E}_{y\sim p(y|x)}[y] = \mathbb{E}[y|x]$. In Bayesian inference, $p(y|x)$ is the posterior distribution, which reflects our updated belief about y after observing evidence x, which is computed via Bayes' Theorem:

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

In Bayesian Flow Networks, a continuous process over time, which transforms a prior distribution into an approximation of the posterior, is applied to learn a conditional distribution $p_\theta(y|x)$ that matches the true distribution.