1 Introduction

1.1 Problem Setup

Suppose $X \in \mathbb{R}^n$ and $Z \in \mathbb{R}^m$ with $X = f(Z) + \varepsilon$, where $f : \mathbb{R}^m \to \mathbb{R}^n$ and $\varepsilon \sim N\left(0, \sigma^2 I\right)$. Assuming Z is normally distributed with independent marginals, this is equivalent to the following latent variable model (a special case of the well-known *nonlinear ICA* model):

$$\begin{aligned} Z &\sim N\left(0, I\right) \\ X \mid Z &\sim N\left(f(Z), \sigma^2 I\right). \end{aligned}$$

Let $\varphi(u; \mu, \Sigma)$ denote the density of a $N(\mu, \Sigma)$ random variable and $p_{\theta,\sigma^2}(x, z)$ denote the joint density under the model. It is easy to see that

$$\begin{aligned} p_{\theta,\sigma^2}\left(x, z\right) &= p_{\theta,\sigma^2}\left(x \mid z\right) p(z) = \varphi\left(x; f(z), \sigma^2 I\right) \varphi(z; 0, I) \\ L\left(\theta, \sigma^2; x\right) &= p_{\theta,\sigma^2}\left(x\right) = \int \varphi\left(x; f(z), \sigma^2 I\right) \varphi(z; 0, I) dz \end{aligned}$$

1.2 Objective Function

Now, suppose we let g_θ denote a family of deep neural network distributions parametrized by θ. To approximate the marginal density $p(x)$, we replace f with g_θ and try to find the choice of θ that maximizes the observed data likelihood. Given k observations $x^{(i)} \overset{i.i.d}{\sim} p(x)$, we wish to solve the following maximum likelihood problem:

$$\max_{\theta,\sigma^2} \underbrace{\sum_{i=1}^{k} \log \int \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz}_{:=\ell(\theta,\sigma^2)}$$

2 Direct MLE Method

In this section, we directly solve the MLE problem by computing gradients of $\ell(\theta, \sigma^2)$ w.r.t θ and σ^2. This is, in general, intractable for arbitrary nonlinear ICA models but worst-case thinking does not apply to our special cases.

Gradient w.r.t θ

$$\begin{aligned} \nabla_\theta \ell(\theta, \sigma^2) &= \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \nabla_\theta \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz \\ &= \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \left(2\pi\sigma^2\right)^{-n/2} \nabla_\theta \exp\left(-\frac{\|x^{(i)} - g_\theta(z)\|_2^2}{2\sigma^2}\right) \varphi(z; 0, I) dz \\ &= \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \nabla_\theta \left(-\frac{\|x^{(i)} - g_\theta(z)\|_2^2}{2\sigma^2}\right) \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz \\ &= \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \left[\frac{1}{\sigma^2} \cdot \left(x^{(i)} - g_\theta(z)\right)^T \nabla_\theta g_\theta(z)\right] \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz \end{aligned}$$

Gradient w.r.t σ^2

$$
\begin{aligned}
\nabla_{\sigma^2}\ell(\theta,\sigma^2) &= \sum_{i=1}^{k} \frac{1}{L\left(\theta,\sigma^2;x^{(i)}\right)} \int \nabla_{\sigma^2}\varphi\left(x^{(i)};g_\theta(z),\sigma^2 I\right)\varphi(z;0,I)dz \\
&= \sum_{i=1}^{k} \frac{1}{L\left(\theta,\sigma^2;x^{(i)}\right)} \int \nabla_{\sigma^2}\left(2\pi\sigma^2\right)^{-n/2}\exp\left(-\frac{\|x^{(i)}-g_\theta(z)\|_2^2}{2\sigma^2}\right)\varphi(z;0,I)dz \\
&= \sum_{i=1}^{k} \frac{1}{L\left(\theta,\sigma^2;x^{(i)}\right)} \int \left[\frac{1}{2\sigma^2}\cdot\left(-n+\frac{\|x^{(i)}-g_\theta(z)\|_2^2}{\sigma^2}\right)\right]\varphi\left(x^{(i)};g_\theta(z),\sigma^2 I\right)\varphi(z;0,I)dz
\end{aligned}
$$

From the two results above, we can iteratively update θ and σ^2 via gradient descent. The integrals can be approximated via numerical integration.

Algorithm 1 Direct MLE via Gradient Descent

- Initialise $\theta^{(0)}$ and $\sigma^{2(0)}$ and set $t=0$
- Repeat until convergence
  - ▷ Compute the gradient $\nabla_\theta \ell\left(\theta^{(t)},\sigma^{2(t)}\right)$ and update the parameters

$$\theta^{(t+1)} = \theta^{(t)} - \eta_1 \nabla_\theta \ell\left(\theta^{(t)},\sigma^{2(t)}\right)$$

  - ▷ Compute the gradient $\nabla_{\sigma^2} \ell\left(\theta^{(t+1)},\sigma^{2(t)}\right)$ and update the parameters

$$\sigma^{2(t+1)} = \sigma^{2(t)} - \eta_2 \nabla_{\sigma^2} \ell\left(\theta^{(t+1)},\sigma^{2(t)}\right)$$

  - ▷ Set $t \leftarrow t+1$

3 Variational Method

In this section, we consider variational inference and VAEs. We use the ELBO to obtain a lower bound on the likelihood $\ell(\theta,\sigma^2)$ and optimize the ELBO using SGD. The marginal likelihoods of individual datapoints can each be rewritten as

$$\log p_\theta\left(x^{(i)}\right) = D_{KL}\left(q_\phi\left(z^{(i)} \mid x^{(i)}\right) \| p_\theta\left(z^{(i)} \mid x^{(i)}\right)\right) + \mathcal{L}\left(\theta,\phi;x^{(i)}\right)$$

The term $\mathcal{L}\left(\theta,\phi;x^{(i)}\right)$ is called the evidence lower bound on the marginal likelihood of datapoint i and can be written as [1]

$$
\begin{aligned}
\log p_\theta\left(x^{(i)}\right) \geq \mathcal{L}\left(\theta,\phi;x^{(i)}\right) &= \mathbb{E}_{q_\phi(z^{(i)}|x^{(i)})}\left[-\log q_\phi\left(z^{(i)} \mid x^{(i)}\right) + \log p_\theta\left(x^{(i)},z^{(i)}\right)\right] \\
&= -D_{KL}\left(q_\phi\left(z^{(i)} \mid x^{(i)}\right) \| p_\theta\left(z^{(i)}\right)\right) + \mathbb{E}_{q_\phi\left(z^{(i)}|x^{(i)}\right)}\left[\log p_\theta\left(x^{(i)} \mid z^{(i)}\right)\right]
\end{aligned}
$$

We want to differentiate and optimize the lower bound $\mathcal{L}\left(\theta, \phi; x^{(i)}\right)$ w.r.t. both the variational parameters ϕ and generative parameters θ. The KL-divergence $D_{KL}\left(q_{\boldsymbol{\phi}}\left(z^{(i)} \mid x^{(i)}\right) \| p_{\boldsymbol{\theta}}\left(z^{(i)}\right)\right)$ can be integrated analytically, such that only the reconstruction error $\mathbb{E}_{q_\phi\left(z^{(i)} \mid x^{(i)}\right)}\left[\log p_\theta\left(x^{(i)} \mid z^{(i)}\right)\right]$ requires estimation by sampling. The *stochastic gradient variational bayes* (SGVB) estimator

$$\widetilde{\mathcal{L}}\left(\theta, \phi; x^{(i)}\right) = -D_{KL}\left(q_\phi\left(z^{(i)} \mid x^{(i)}\right) || p_\theta\left(z^{(i)}\right)\right) + \frac{1}{L}\sum_{l=1}^{L} \log p_\theta\left(x^{(i)} \mid z^{(i,l)}\right)$$

KL-divergence

When both the prior $p_\theta(z) = \mathcal{N}(0, I)$ and the posterior approximation $q_\phi\left(z^{(i)} \mid x^{(i)}\right)$ are Gaussian, the KL term that can be integrated analytically. Let J be the dimensionality of z. Let μ and σ denote the variational mean and std evaluated at datapoint i, and let μ_j and σ_j denote the j-th element of these vectors.

$$\begin{aligned} -D_{KL}\left(q_\phi(z \mid x) \| p_\theta(z)\right) &= \int q_\phi(z \mid x)\left(\log p_\theta(z) - \log q_\phi(z \mid x)\right) dz \\ &= \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log\left((\sigma_j)^2\right) - (\mu_j)^2 - (\sigma_j)^2\right) \end{aligned}$$

Probabilistic encoders and decoders

In variational auto-encoders, neural networks are used as probabilistic encoders and decoders. For both the encoder and decoder, we use a MLP with Gaussian outputs. Let the decoder be a multivariate Gaussian with a diagonal covariance structure

$$\begin{aligned} \log p\left(x \mid z\right) &= \log \mathcal{N}\left(x; m, s^2 I\right) \\ \text{where } h &= h\left(z\right) \\ m &= W_1 h + b_1 \\ \log s^2 &= W_2 h + b_2 \end{aligned}$$

where $\{W_1, W_2, b_1, b_2\}$ are the weights and biases of the MLP (as part of θ) with $m \in R^n$ and $s^2 \in R$. The reconstruction error can be expanded as

$$\log p\left(x \mid z\right) = -\frac{n}{2} \cdot \log\left(2\pi s^2\right) - \frac{\|x - m\|_2^2}{2s^2}$$

[1] An equivalent concept to ELBO is the variational free energy. The variational free energy in a latent variable model $p_\theta(x, z)$ is defined as

$$\mathcal{L}(\theta, q) = \mathbb{E}_{z \sim q}\left[-\log q(z) + \log p_\theta(x, z)\right],$$

where q is any probability density/mass function over the latent variables z. The first term is the Shannon entropy $H(q) = -\mathbb{E}_{z \sim q} \log q(z)$ of the variational distribution $q(z)$ and does not depend on θ. The second term is sometimes referred to as the energy.