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):

$$Z \sim N(0, I)$$
$$X \mid Z \sim N\left(f(Z), \sigma^2 I\right).$$

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

$$p_{\theta, \sigma^2}(x, z) = p_{\theta, \sigma^2}(x \mid z) \, p(z) = \varphi\left(x; f(z), \sigma^2 I\right) \varphi(z; 0, I)$$

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

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

$$\nabla_\theta \ell(\theta, \sigma^2) = \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \nabla_\theta \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz$$

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

$$= \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \nabla_\theta \left(-\frac{\|x^{(i)} - g_\theta(z)\|_2^2}{2\sigma^2}\right) \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz$$

$$= \sum_{i=1}^{k} \frac{1}{L\left(\theta, \sigma^2; x^{(i)}\right)} \int \left[\frac{1}{\sigma^2} \cdot \left(x^{(i)} - g_\theta(z)\right)^T \nabla_\theta g_\theta(z)\right] \varphi\left(x^{(i)}; g_\theta(z), \sigma^2 I\right) \varphi(z; 0, I) dz$$

Gradient w.r.t σ^2

$$\nabla_{\sigma^2}\ell(\theta,\sigma^2) = \sum_{i=1}^{k} \frac{1}{L\left(\theta,\sigma^2;x^{(i)}\right)} \int \nabla_{\sigma^2}\varphi\left(x^{(i)};g_\theta(z),\sigma^2 I\right)\varphi(z;0,I)dz$$

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

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

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 $t \leftarrow t+1$

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3 Variational Method

In this section, we consider variational inference and VAEs. We use the ELBO to obtain a lower bound on the likelihood $\ell(\theta,\sigma)$ 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]

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

$$= -D_{KL}\left(q_\phi\left(z^{(i)}\mid x^{(i)}\right)\|p_\theta\left(z^{(i)}\right)\right) + \mathbb{E}_{q_\phi(z^{(i)}|x^{(i)})}\left[\log p_\theta\left(x^{(i)}\mid z^{(i)}\right)\right]$$

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 $D_{KL}\left(q_\phi\left(z^{(i)} \mid x^{(i)}\right) \| p_{\boldsymbol{\theta}}(z^{(i)})\right)$ 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.

$$-D_{KL}\left(q_\phi(z) \| p_\theta(z)\right) = \int q_\phi(z)\left(\log p_\theta(z) - \log q_\phi(z)\right) dz$$

$$= \frac{1}{2} \sum_{j=1}^{J}\left(1 + \log\left((\sigma_j)^2\right) - (\mu_j)^2 - (\sigma_j)^2\right)$$

Probabilistic encoders and decoders

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

$$\log p\left(x \mid z\right) = \log \mathcal{N}\left(x; \mu, \sigma^2, I\right)$$
$$\text{where } h = h\left(z\right)$$
$$\mu = W_1 h + b_1$$
$$\log \sigma^2 = W_2 h + b_2$$

where $\{W_1, W_2, b_1, b_2\}$ are the weights and biases of the MLP (as part of θ).

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[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 $H(q) = -\mathbb{E}_q \log q(z)$ of the variational distribution $q(z)$, and does not depend on θ. The second term is sometimes referred to as the energy.