

MLE/VAE for nonlinear ICA

1 Introduction

1.1 Problem Setup

Suppose $X \in \mathbb{R}^n$ and $Z \in \mathbb{R}^m$ with $X = f(Z) + \varepsilon$, where $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$ and $\varepsilon \sim N(0, \sigma^2 I)$. 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):

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

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

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

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 $x^{(i)} \stackrel{i.i.d}{\sim} p(x)$, we wish to solve the following maximum likelihood problem:

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

1.3 Nonlinear ICA [1]

Now we show how the model above is closely related to previous work on nonlinear ICA. In nonlinear ICA, we assume observations $x \in \mathbb{R}^d$, which are the result of an unknown (but invertible) transformation f of latent variables $z \in \mathbb{R}^d$:

$$x = f(z)$$

where z are assumed to follow a factorized (but typically unknown) distribution $p(z) = \prod_{i=1}^d p_i(z_i)$. This model is essentially a deep generative model.

The difference to the definition above is mainly in the lack of noise and the equality of the dimensions: the transformation f is deterministic and invertible. Thus, any posteriors would be degenerate. The goal is then to recover (identify) f^{-1} , which gives the independent components as $z = f^{-1}(x)$, based on a dataset of observations of x alone.

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

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

Gradient w.r.t σ^2

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

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

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

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

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

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

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

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

KL-divergence

When both the prior $p_{\theta}(z) = \mathcal{N}(0, I)$ and the posterior approximation $q_{\phi}(z^{(i)} | x^{(i)})$ 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.

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

Reconstruction Error

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

¹An 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

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

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.

multivariate Gaussian with a diagonal covariance structure

$$\log p(x | z) = \log \mathcal{N}(x; m, s^2 I)$$

$$\text{where } h = h(z)$$

$$m = W_1 h + b_1$$

$$\log s^2 = W_2 h + b_2$$

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

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

References

- [1] Khemakhem, Ilyes, et al. “Variational Autoencoders and Nonlinear ICA: A Unifying Framework.” ArXiv.org, 21 Dec. 2020, arxiv.org/abs/1907.04809.
- [2] Kingma, Diederik P., and Max Welling. “An Introduction to Variational Autoencoders.” ArXiv.org, 11 Dec. 2019, <https://arxiv.org/abs/1906.02691>.
- [3] Kingma, Diederik P, and Max Welling. “Auto-Encoding Variational Bayes.” ArXiv.org, 1 May 2014, <https://arxiv.org/abs/1312.6114>.