The Reparamaterisation Trick

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Abstract

The reparamatisation trick is used to enable variational autoencoders (VAEs) to be trained with gradient descent.

1 Quick Overview of Variational Autoencoders

Let $\mathbf{z}$ be a vector of latent variables, $\mathbf{x}$ be a row vector from a dataset X, $q_\phi(\mathbf{z}|\mathbf{x})$ be the encoder and $p_\theta(\mathbf{x}|\mathbf{z})$ be the decoder. The loss function used is referred to as the evidence lower bound (ELBO). ELBO is defined as follows

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = log(p_\theta(\mathbf{x})) - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})) \tag{1}$$

where D_{KL} is the Kullback-Leibler divergence.

1.1 More on ELBO

`https://www.zinkov.com/posts/2018-11-02-decomposing-the-elbo/`

2 Optimising ELBO with SGD

To optimise our VAE, we need to be able to take gradients of the expected value of ELBO with respect to the network weights θ and ϕ. This is easy enough for θ:

$$\nabla_\theta \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\mathcal{L}_{\theta,\phi}(\mathbf{x})] = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\nabla_\theta \mathcal{L}_{\theta,\phi}(\mathbf{x})] \tag{2}$$

Once the grad operator is inside the expectation, all we have to do is approximate the expectation with a sample.

Things are trickier with ϕ. As the expectation assumes that $p(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}|\mathbf{x})$, we cannot simply move ∇_ϕ in and out of the expectation arbitrarily.

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\mathcal{L}_{\theta,\phi}(\mathbf{x})] \neq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\nabla_\phi \mathcal{L}_{\theta,\phi}(\mathbf{x})] \tag{3}$$

That the left and right hand sides are not equal can be seen as follows:

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\mathcal{L}_{\theta,\phi}(\mathbf{x})] = \nabla_\phi \int q_\phi(\mathbf{z}|\mathbf{x})\mathcal{L}_{\theta,\phi}(\mathbf{x})d\mathbf{x} \tag{4}$$

$$= \int \nabla_\phi (q_\phi(\mathbf{z}|\mathbf{x})\mathcal{L}_{\theta,\phi}(\mathbf{x}))d\mathbf{x} \tag{5}$$

$$= \int [q_\phi(\mathbf{z}|\mathbf{x})(\nabla_\phi \mathcal{L}_{\theta,\phi}(\mathbf{x})) + \mathcal{L}_{\theta,\phi}(\mathbf{x})(\nabla_\phi q_\phi(\mathbf{z}|\mathbf{x}))]d\mathbf{x} \tag{6}$$

$$= \int q_\phi(\mathbf{z}|\mathbf{x})(\nabla_\phi \mathcal{L}_{\theta,\phi}(\mathbf{x}))d\mathbf{x} + \int \mathcal{L}_{\theta,\phi}(\mathbf{x})(\nabla_\phi q_\phi(\mathbf{z}|\mathbf{x}))d\mathbf{x} \tag{7}$$

$$= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\nabla_\phi \mathcal{L}_{\theta,\phi}(\mathbf{x})] + \int \mathcal{L}_{\theta,\phi}(\mathbf{x})(\nabla_\phi q_\phi(\mathbf{z}|\mathbf{x}))d\mathbf{x} \tag{8}$$

This isn't in a form that we can easily handle. In particular, $\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})$, meaning $\mathbf{z}$ is stochastic rather than deterministic. This is where the reparamaterisation trick comes into play. We can make $\mathbf{z}$ deterministic by making it a function of a stochastic variable, ϵ:

$$\mathbf{z} = g(\epsilon, \phi, \mathbf{x}) \tag{9}$$

After replacing $\mathbf{z}$ with $g(\epsilon, \phi, \mathbf{x})$, the expectation is then taken over the distribution of ϵ. The stochasticity is now separated from θ, allowing us to calculate $\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\mathcal{L}_{\theta,\phi}(\mathbf{x})]$ as follows:

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\mathcal{L}_{\theta,\phi}(\mathbf{x})] = \nabla_\phi \mathbb{E}_{p(\epsilon)}[\mathcal{L}_{\theta,\phi}(\mathbf{x})] \tag{10}$$

$$= \mathbb{E}_{p(\epsilon)}[\nabla_\phi \mathcal{L}_{\theta,\phi}(\mathbf{x})] \tag{11}$$

References

[1] Carl Doersch, *Tutorial on variational autoencoders*, 2016.

[2] Diederik P. Kingma and Max Welling, *An introduction to variational autoencoders*, 2019.