Variational Autoencoders

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Simplification

For ease of illustration, we restrict our attention to a variational autoencoder that applies i.i.d assumptions and Gaussian distributions (and therefore real-valued observations) throughout. Note that neither assumption is necessary.

Probabilistic decoder

Consider a parametric frequentist latent variable model, with

- observations $x = (x^{(i)})_{i=1}^N, \quad x^{(i)} \in \mathbb{R}^d$
- latent variables $z = (z^{(i)})_{i=1}^N, \quad z^{(i)} \in \mathbb{R}^k$
- parameter θ (fixed but to be learned)

Let us model our observations x via the factorization

$$p_\theta(x|z) = \prod_i p_\theta(x^{(i)}|z^{(i)})$$

Let the likelihood of each observation $x^{(i)}$ be obtained by using a Multi-Layer Perceptron (MLP), parameterized by weights θ, to map latent variable $z^{(i)}$ to Gaussian parameters governing the distribution of observation $x^{(i)}$.

$$x^{(i)}|z^{(i)}, \theta \sim \mathcal{N}\left(\mu_{x^{(i)}}(z^{(i)}; \theta),\ \Sigma_{x^{(i)}}(z^{(i)}; \theta)\right) \tag{2.1}$$

Since the MLP maps latent variables, z, to the parameters of a probability distribution over observed data, x, we refer to it as a **probabilistic decoder.**

Notes on notation

1. $\mathcal{N}(M, V)$ refers to the Gaussian density with mean M and covariance V.
2. $\mu_{x^{(i)}}(z^{(i)}; \theta)$ is meant to denote the mean parameter for a distribution over observed datum $x^{(i)}$; that parameter is a function of latent variable z and learnable parameter θ. Notation should be similarly interpreted throughout this section.

Probabilistic encoder

Let us additionally put a prior distribution on the latent variables:

$$p_\theta(z) = \prod_i p_\theta(z^{(i)}) = \prod_i \mathcal{N}(\mathbf{0}, \mathbb{I})$$

In this case, the posterior distribution, $p_\theta(z|x)$, is intractable. However, we consider an approximation by using a Multi-Layer Perceptron (MLP), parameterized by weights ϕ, to map observation x to Gaussian parameters governing the distribution of latent variable z:

$$\begin{aligned} q_\phi(z|x) &= \prod_i \; q_\phi(z^{(i)}|x^{(i)}) \\ z^{(i)}|x^{(i)}, \phi &\sim \mathcal{N}\left(\mu_{z^{(i)}}(x^{(i)}; \phi), \Sigma_{z^{(i)}}(x^{(i)}; \phi)\right) \end{aligned} \tag{2.2}$$

Since the MLP maps observations, x, to to the parameters of a probability distribution over latent variables, z, we refer to it as a **probabilistic encoder.**

Probabilistic encoder

- We may regard the probabilistic encoder as an approximation to the posterior distribution over latent variables which results from using the probabilistic decoder as a likelihood.
- The probabilistic encoder is sometimes also referred to as a **recognition model**.

Sample Implementation

Sample Implementation

Following Appendix C.2 of the VAE paper, we provide a sample implementation for the probabilistic encoder and decoder.

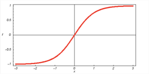
Probabilistic encoding

We may, for example, specifically assume that an observation $x^{(i)}$ can be probabilistically encoded into latent variable $z^{(i)}$ via the following process

$$h^{(i)} = \mathtt{tanh}(W_1 x^{(i)} + b_1)$$

$$\mu_{z^{(i)}} = W_{21} h^{(i)} + b_{21}, \quad \log \sigma^2_{z^{(i)}} = W_{22} h^{(i)} + b_{22}$$

$$z^{(i)} \sim \mathcal{N}(\mu_{z^{(i)}}, \Sigma_{z^{(i)}}), \quad \text{where } \operatorname{diag}(\Sigma_{z^{(i)}}) = \sigma^2_{z^{(i)}}$$



The hyperbolic tangent (tanh) function

where (W_1, W_{21}, W_{22}) are the weights and (b_1, b_{21}, b_{22}) are the biases of a Multi-Layer Perceptron (MLP).

Letting $\phi := (W_1, W_{21}, W_{22}, b_1, b_{21}, b_{22})$, we may use the trained encoder to define the approximate posterior, $q_\phi(z|x)$, as defined in (2.2).

Probabilistic decoding

We may, for example, specifically assume that a latent variable $z^{(i)}$ can be probabilistically decoded into observation $x^{(i)}$ via the following process

$$
\begin{aligned}
h^{(i)} &= \texttt{tanh}(W_3\, z^{(i)} + b_3) \\
\mu_{x^{(i)}} &= W_{41} h^{(i)} + b_{41}, \quad \log \sigma^2_{x^{(i)}} = W_{42} h^{(i)} + b_{42} \\
x|z &\sim \mathcal{N}(\mu_{x^{(i)}}, \Sigma_{x^{(i)}}), \quad \text{where } \operatorname{diag}(\Sigma_{x^{(i)}}) = \sigma^2_{x^{(i)}}
\end{aligned}
$$

where (W_3, W_{41}, W_{42}) are the weights and (b_3, b_{41}, b_{42}) are the biases of a Multi-Layer Perceptron (MLP).

Letting $\theta := (W_3, W_{41}, W_{42}, b_3, b_{41}, b_{42})$, we may use the trained decoder to define the likelihood, $p_\theta(x|z)$, as defined in (2.1).

Inference

We use variational inference to jointly optimize (θ, ϕ). For example, in our sample implementation, we have

$$\begin{aligned} \theta &= (W_3, W_{41}, W_{42}, b_3, b_{41}, b_{42}) && \text{generative parameters} \\ \phi &= (W_1, W_{21}, W_{22}, b_1, b_{21}, b_{22}) && \text{variational parameters} \end{aligned}$$

In particular, we construct $\mathcal{F}(\theta, \phi; x)$, a lower-bound on the marginal likelihood, $p_\theta(x)$, via the entropy/energy decomposition which is standard in variational inference:

$$\mathcal{F}(\theta, \phi; x) = \mathbb{E}_{q_\phi(z|x)}[-\log q_\phi(z|x)) + \log p_\theta(x, z)] \tag{4.1}$$

We train the model by performing stochastic gradient descent on the variational lower bound $\mathcal{F}$. During training, the objective function (4.1) is approximated by performing a Monte Carlo approximation of the expectation. Given minibatch $x^{(i)}$, we would like to take L samples from $q_\phi(z|x^{(i)})$ and obtain the following estimator:

$$\mathcal{F}(\theta, \phi; x^{(i)}) \approx \frac{1}{L} \sum_{l=1}^{L} - \log q_\phi(z^{(i,l)}|x^{(i)}) + \log p_\theta(x^{(i)}, z^{(i,l)}) \qquad (4.2)$$

However, naively backpropagating gradients in this case would ignore the role of the parameter in the sampling step. Thus, we use the **reparameterization trick** ; i.e. we construct a differentiatiable transformation g_ϕ of parameterless distribution $p(\epsilon)$ such that $g_\phi(\epsilon, x^{(i)})$ has the same distribution as $q_\phi(z^{(i)}|x^{(i)})$.[1] Using this trick, we take L samples $\{\epsilon_1, ..., \epsilon_L\}$ from $p(\epsilon)$ and obtain the estimator:

$$\mathcal{F}(\theta, \phi; x^{(i)}) \approx \frac{1}{L} \sum_{l=1}^{L} - \log q_\phi\big(g_\phi(\epsilon^{(l)}, x^{(i)})|x^{(i)}\big) + \log p_\theta\big(x^{(i)}, g_\phi(\epsilon^{(l)}, x^{(i)})\big) \tag{4.3}$$

[1] In this case, since our variational distribution is a multivariate normal, $p(\epsilon)$ is simply a Gaussian with zero mean and identity covariance.

Anomaly Scoring

Anomaly Scoring

A straightforward approach to assessing anomalousness of sample $x^{(i)}$ using a Variational Autoencoder was provided by the authors below. First, take L samples, $\{z^{(i,1)}, ..., z^{(i,L)}\}$ from the fitted variational distribution (i.e, the encoder), $q_\phi(z^{(i)}|x^{(i)})$. Each such sample, $z^{(i,l)}$, determines a specific form of the fitted likelihood (i.e. the decoder) by specifying its parameters, $p_\theta(x^{(i)}|z^{(i,l)}) = p_\theta(x^{(i)}|\mu_{x^{(i)}}(z^{(i,l)}), \Sigma_{x^{(i)}}(z^{(i,l)}))$. Using this, the *reconstruction probability* of the sample can be defined as the mean of these likelihoods:

$$\texttt{reconstruction probability}(x^{(i)}) := \frac{1}{L}\sum_{l=1}^{L} p_\theta\left(x^{(i)} \mid \mu_{x^{(i)}}(z^{(i,l)}) , \Sigma_{x^{(i)}}(z^{(i,l)})\right)$$

An, J., & Cho, S. (2015). Variational autoencoder based anomaly detection using reconstruction probability. Special Lecture on IE, 2(1).