Variational Autoencoders

Kingma et al. (2014)

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Review of Variational Inference

Setting:

x is our data.
z is our latent variable.
Joint density is $p(x, z) = p(x|z) \cdot (z)$

Goal: Approximate the posterior $p(z|x) = \frac{p(x|z)p(z)}{p(x)}$,
where marginal $p(x) = \int p(x|z)p(z)dz$ is intractible.

Strategy: We pose a family of approximations, Q, and choose a member of that family, $q(z) \in Q$, to minimize $KL\left[q(z)||p(z|x)\right]$.

Review of Variational Inference (2)

We want to find the best approximation:

$$q^*(z) = \underset{q(z) \in Q}{\arg\min}\, KL\left[q(z)||p(z|x)\right]$$

This objective is intractible because it involves $p(x)$:

$$\begin{aligned} KL\left[q(z)||p(z|x)\right] &= E_{q(z)}\left[log\left(\frac{q(z)}{p(z|x)}\right)\right] \\ &= E_{q(z)}\left[log\left(q(z)\right)\right] - E_{q(z)}\left[log\left(p(x,z)\right)\right] + log\left(p(x)\right) \end{aligned}$$

Review of Variational Inference (3)

We can maximize another quantity which is equivalent to minimizing the KL divergence. (The $log\left(p(x)\right)$ term is constant wrt $q(z)$.)

$$KL\left[q(z)||p(z|x)\right] = \underbrace{E_{q(z)}\left[log\left(q(z)\right)\right] - E_{q(z)}\left[log\left(p(x,z)\right)\right]}_{-ELBO(q)} + log\left(p(x)\right)$$

We can write $ELBO(q)$ as

$$\begin{aligned} ELBO(q) &= E_{q(z)}\left[log\left(q(z)\right)\right] - E_{q(z)}\left[log\left(p(x,z)\right)\right] \\ &= E_{q(z)}\left[log\left(p(z)\right)\right] + E_{q(z)}\left[log\left(p(x|z)\right)\right] - E_{q(z)}\left[log\left(q(z)\right)\right] \\ &= E_{q(z)}\left[log\left(p(x|z)\right)\right] - KL\left[q(z)||p(z)\right] \end{aligned}$$

The $ELBO(q)$ is a lower bound on $log\left(p(x)\right)$.

Variational Auto Encoders: Notation Note

Going forward, we will write $q(z)$ as $q(z|x)$.

We will also add a subscript to indicate that $q(z|x)$ is parameterized by variational parameters labeled ϕ.

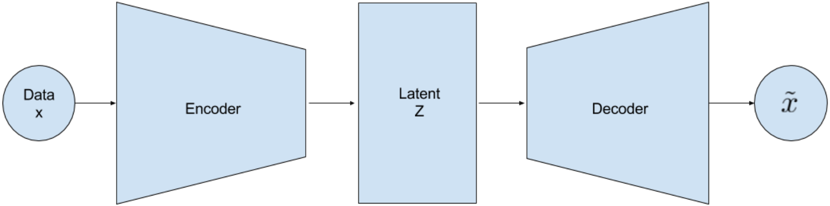
We write: $q_\phi(z|x)$

Purpose of VAEs

What do VAEs do?

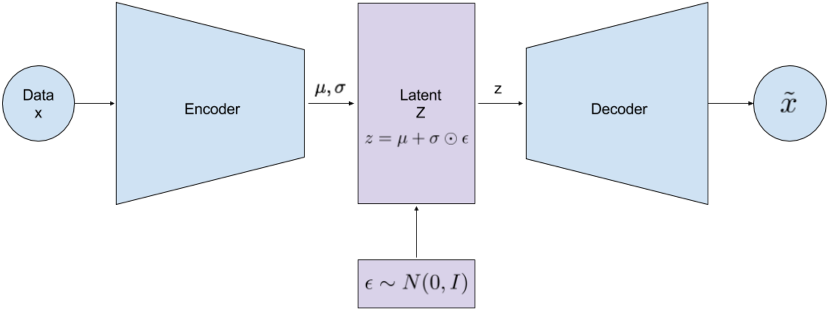
- Fit a generative model to a large dataset.
- Model the underlying distribution of the data and sample new data from the distribution.
- Image re-generation, and generating new images like existing ones.

Basic VAE Setup



In neural nets language, a VAE consists of an encoder, a decoder, and a loss function.

The Latent Variables



- Latent z is a continuous, lower-dimensional; dimension is a user input.
- Let the prior $p(z)$ be isotropic multivariate Gaussian: $p(z) \sim N(z; \mathbf{0}, \mathbf{I})$.

The Latent Variables: Reparameterization Trick

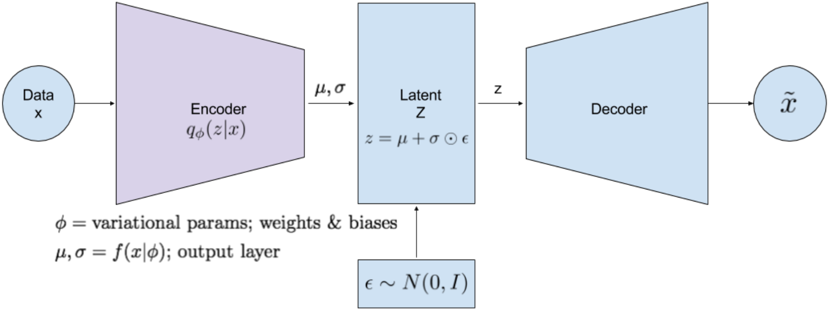
Why use $z = \mu + \sigma \odot \epsilon, \epsilon \sim N(0, I)$ instead of sampling $z \sim N(\mu, \sigma I)$?

We must remove the randomness from the neural networks in order to use back-propogation with stochastic gradient descent to train.

Interpretation of σ:

- Think of z as encoding information in a lower-dimensional space. How to prevent encoding an infinite amount of info?
- What if we have two x's which are very different, mapped to two z's which are close?
- σ acts as noise, which prevents reconstructing two different $\tilde{x}$ values from z's which are less than σ apart. Regulates how much info you can encode.

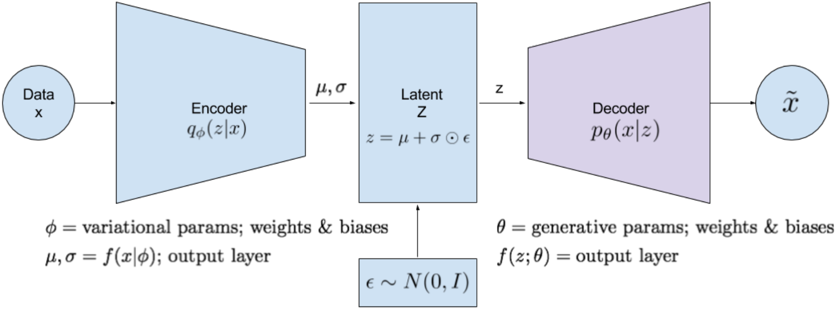
The Encoder



ϕ = variational params; weights & biases

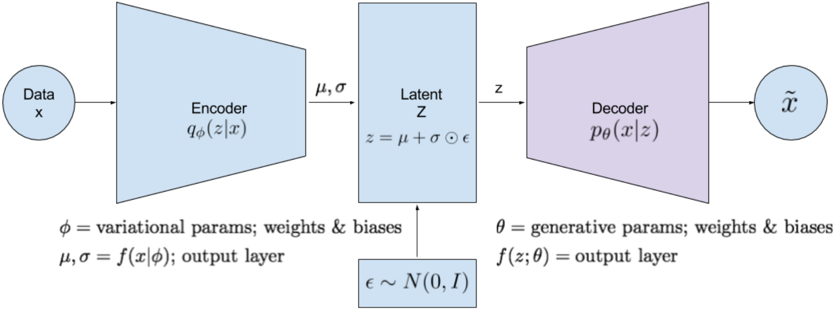
$\mu, \sigma = f(x|\phi)$; output layer

The Decoder


Data
x
Encoder
$q_\phi(z|x)$
μ, σ
Latent
Z
$z = \mu + \sigma \odot \epsilon$
z
Decoder
$p_\theta(x|z)$
$\tilde{x}$
ϕ = variational params; weights & biases
$\mu, \sigma = f(x|\phi)$; output layer
$\epsilon \sim N(0, I)$
θ = generative params; weights & biases
$f(z;\theta)$ = output layer

The Decoder

$$p_\theta(x|z) \sim N\left(f(z;\theta), \sigma^2 I\right)$$
$$p_\theta(x|z) \sim Bernoulli\left(f\left(z;\theta\right)\right)$$



Training the Model

Model parameters (ϕ, θ) are trained using stochastic gradient descent with back-propogation.

- (ϕ, θ) are learned jointly.
- With step size ρ, encoder and decoder parameters are updated as

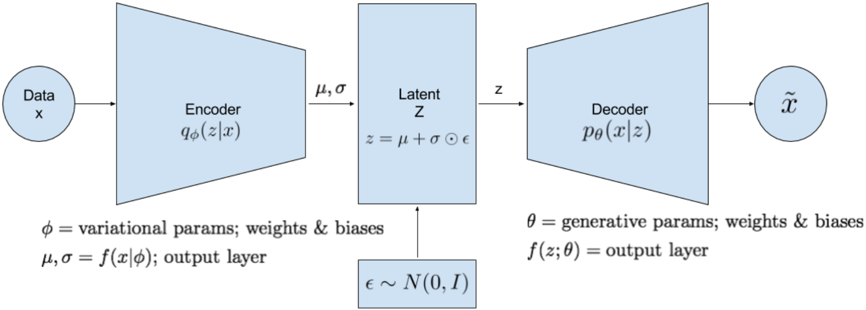
$$\phi_{\mathsf{new}} = \phi_{\mathsf{old}} - \rho \frac{\partial L_i(\phi, \theta, x_i)}{\partial \phi}$$

$$\theta_{\mathsf{new}} = \theta_{\mathsf{old}} - \rho \frac{\partial L_i(\phi, \theta, x_i)}{\partial \theta}$$

where $L_i(\phi, \theta, x_i)$ is a loss function.

The Loss Function

$$p_\theta(x|z) \sim N\left(f(z;\theta), \sigma^2 I\right)$$
$$p_\theta(x|z) \sim Bernoulli\left(f\left(z;\theta\right)\right)$$



$$L(\phi, \theta, x) = -ELBO_q(\phi, \theta, x) = -E_{q_\phi(z|x)}\left[log p_\theta(x|z)\right] + KL\left[q_\phi(z|x)||p(z)\right]$$

Tasks we can accomplish after training

(1) Inference on parameters (the Gaussian means, or Bernoulli probabilities).

(2) Efficient approximation of posterior of latent z given observed x for a set of parameters. (Coding tasks, data representation)

(3) Efficient approximate marginal inference of x:

- Reconstruct data sets we have seen.
- Generate new data sets that are like one we have already seen.

Sampling of papers

- Variational Autoencoder for Deep Learning of Images, Labels and Captions
- Alternative priors for Deep Generative Models
- Least Squares VAE with Regularization
- Stein VAE
- Ladder VAEs

Example on github

In the example on github:

- Uses the MNIST data set.
- Uses a gaussian encoder and a bernoulli decoder.
- Both neural nets have two hidden layers.
- Uses drop-outs (tf.nn.dropout) to avoid overfitting.