COMS 4995 Lecture 13: Variational Autoencoders

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Overview

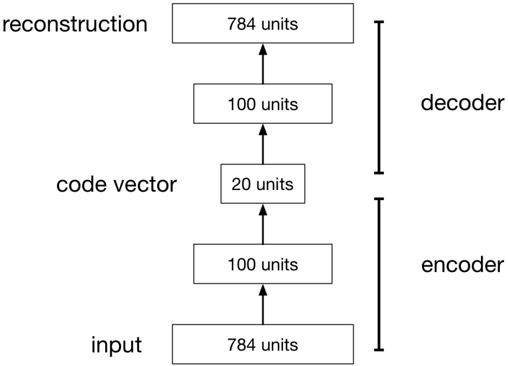
Four modern approaches to generative modeling:

- Autoregressive models
- Generative adversarial networks
- Reversible architectures
- Variational autoencoders (this lecture)

All four approaches have different pros and cons.

Autoencoders

- An autoencoder is a feed-forward neural net whose job it is to take an input **x** and predict **x**.
- To make this non-trivial, we need to add a bottleneck layer whose dimension is much smaller than the input.



Autoencoders

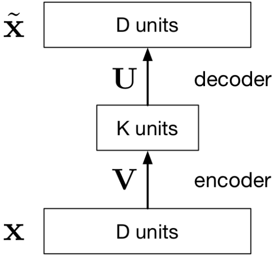
Why autoencoders?

- Map high-dimensional data to two dimensions for visualization
- Compression (i.e. reducing the file size)
- Learn abstract features in an unsupervised way so you can apply them to a supervised task
  - Unlabled data can be much more plentiful than labeled data
- Learn a semantically meaningful representation where you can, e.g., interpolate between different images.

Principal Component Analysis (optional)

- The simplest kind of autoencoder has one hidden layer, linear activations, and squared error loss.

$$\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|^2$$



- This network computes $\tilde{\mathbf{x}} = \mathbf{U}\mathbf{V}\mathbf{x}$, which is a linear function.
- If $K \geq D$, we can choose $\mathbf{U}$ and $\mathbf{V}$ such that $\mathbf{U}\mathbf{V}$ is the identity. This isn't very interesting.
- But suppose $K < D$:
  - $\mathbf{V}$ maps $\mathbf{x}$ to a K-dimensional space, so it's doing dimensionality reduction.
  - The output must lie in a K-dimensional subspace, namely the column space of $\mathbf{U}$.

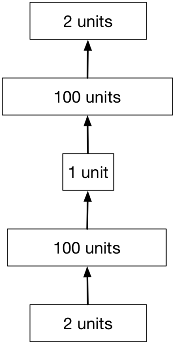
Principal Component Analysis (optional)

- Linear autoencoders with squared error loss are equivalent to Principal Component Analysis (PCA).
- Two equivalent formulations:
  - Find the subspace that minimizes the reconstruction error.
  - Find the subspace that maximizes the projected variance.
- The optimal subspace is spanned by the dominant eigenvectors of the empirical covariance matrix.

“Eigenfaces”

Deep Autoencoders

- Deep nonlinear autoencoders learn to project the data, not onto a subspace, but onto a nonlinear manifold
- This manifold is the image of the decoder.
- This is a kind of nonlinear dimensionality reduction.



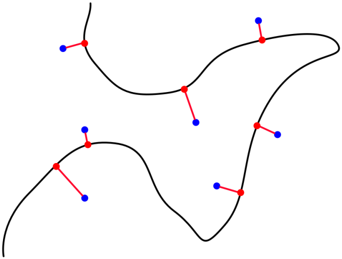
2 units

100 units

1 unit

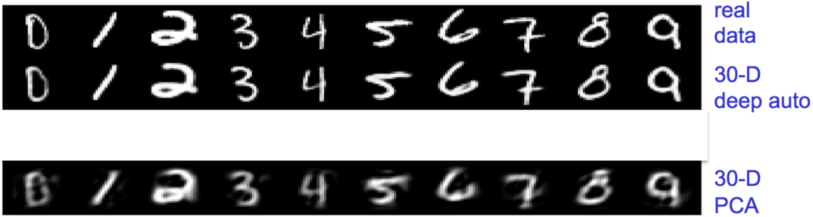
100 units

2 units



Deep Autoencoders

- Nonlinear autoencoders can learn more powerful codes for a given dimensionality, compared with linear autoencoders (PCA)



Deep Autoencoders

- Some limitations of autoencoders
  - They're not generative models, so they don't define a distribution
  - How to choose the latent dimension?

Observation Model

- Consider training a generator network with maximum likelihood.

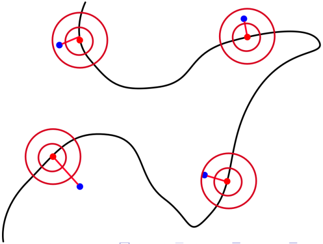
$$p(\mathbf{x}) = \int p(\mathbf{z}) p(\mathbf{x} \mid \mathbf{z}) \, \mathrm{d}\mathbf{z}$$

- One problem: if $\mathbf{z}$ is low-dimensional and the decoder is deterministic, then $p(\mathbf{x}) = 0$ almost everywhere!
  - The model only generates samples over a low-dimensional sub-manifold of $\mathcal{X}$.

- Solution: define a noisy observation model, e.g.

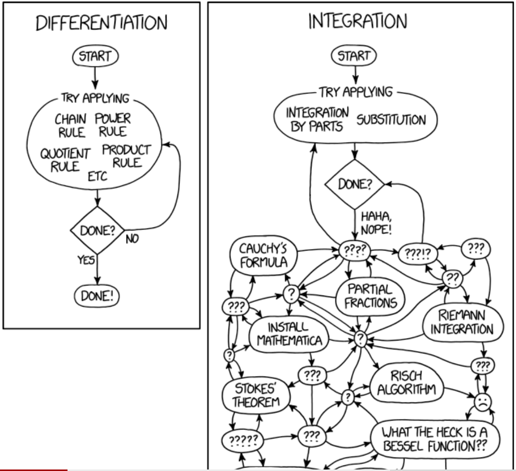
$$p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mathbf{x}; G_{\boldsymbol{\theta}}(\mathbf{z}), \eta \mathbf{I}),$$

where $G_{\boldsymbol{\theta}}$ is the function computed by the decoder with parameters $\boldsymbol{\theta}$.



Observation Model

- At least $p(\mathbf{x}) = \int p(\mathbf{z}) p(\mathbf{x} \,|\, \mathbf{z}) \, \mathrm{d}\mathbf{z}$ is well-defined, but how can we compute it?
- Integration, according to XKCD:



Observation Model

- At least $p(\mathbf{x}) = \int p(\mathbf{z})p(\mathbf{x} \mid \mathbf{z})\,\mathrm{d}\mathbf{z}$ is well-defined, but how can we compute it?
  - The decoder function $G_{\boldsymbol{\theta}}(\mathbf{z})$ is very complicated, so there's no hope of finding a closed form.
- Instead, we will try to maximize a lower bound on $\log p(\mathbf{x})$.
  - The math is essentially the same as for the EM algorithm.

Variational Inference

- We obtain the lower bound using Jensen's Inequality: for a convex function h of a random variable X,

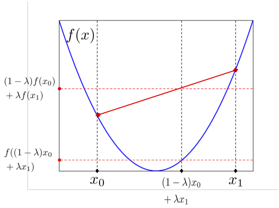
$$\mathbb{E}[h(X)] \geq h(\mathbb{E}[X])$$

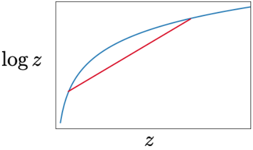
Therefore, if h is concave (i.e. $-h$ is convex),

$$\mathbb{E}[h(X)] \leq h(\mathbb{E}[X])$$

- The function $\log z$ is concave. Therefore,

$$\mathbb{E}[\log X] \leq \log \mathbb{E}[X]$$





Variational Inference

- Suppose we have some distribution $q(\mathbf{z})$. (We'll see later where this comes from.)
- We use Jensen's Inequality to obtain the lower bound.

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log \int p(\mathbf{z})\, p(\mathbf{x}|\mathbf{z})\, \mathrm{d}\mathbf{z} \\
&= \log \int q(\mathbf{z})\, \frac{p(\mathbf{z})}{q(\mathbf{z})} p(\mathbf{x}|\mathbf{z})\, \mathrm{d}\mathbf{z} \\
&\geq \int q(\mathbf{z}) \log \left[\frac{p(\mathbf{z})}{q(\mathbf{z})}\, p(\mathbf{x}|\mathbf{z}) \right] \mathrm{d}\mathbf{z} \qquad \text{(Jensen's Inequality)} \\
&= \mathbb{E}_q \left[\log \frac{p(\mathbf{z})}{q(\mathbf{z})} \right] + \mathbb{E}_q \left[\log p(\mathbf{x}|\mathbf{z}) \right]
\end{aligned}
$$

- We'll look at these two terms in turn.

Variational Inference

- The first term we'll look at is $\mathbb{E}_q\left[\log p(\mathbf{x}|\mathbf{z})\right]$
- Since we assumed a Gaussian observation model,

$$\begin{aligned}\log p(\mathbf{x}|\mathbf{z}) &= \log \mathcal{N}(\mathbf{x}; G_{\boldsymbol{\theta}}(\mathbf{z}), \eta \mathbf{I}) \\ &= \log \left[\frac{1}{(2\pi\eta)^{D/2}} \exp\left(-\frac{1}{2\eta} \|\mathbf{x} - G_{\boldsymbol{\theta}}(\mathbf{z})\|^2 \right) \right] \\ &= -\frac{1}{2\eta} \|\mathbf{x} - G_{\boldsymbol{\theta}}(\mathbf{z})\|^2 + \text{const}\end{aligned}$$

- So this term is the expected squared error in reconstructing $\mathbf{x}$ from $\mathbf{z}$. We call it the reconstruction term.

Variational Inference

- The second term is $\mathbb{E}_q \left[\log \frac{p(\mathbf{z})}{q(\mathbf{z})} \right]$.
- This is just $-\mathrm{D}_{\mathrm{KL}}(q(\mathbf{z}) \| p(\mathbf{z}))$, where D_{KL} is the Kullback-Leibler (KL) divergence

$$\mathrm{D}_{\mathrm{KL}}(q(\mathbf{z}) \| p(\mathbf{z})) \triangleq \mathbb{E}_q \left[\log \frac{q(\mathbf{z})}{p(\mathbf{z})} \right]$$

  - KL divergence is a widely used measure of distance between probability distributions, though it doesn't satisfy the axioms to be a distance metric.
  - More details in tutorial.
- Typically, $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$. Hence, the KL term encourages q to be close to $\mathcal{N}(\mathbf{0}, \mathbf{I})$.
- We'll give the KL term a much more interesting interpretation when we discuss Bayesian neural nets.

Variational Inference

- Hence, we're trying to maximize the variational lower bound, or variational free energy:

$$\log p(\mathbf{x}) \geq \mathcal{F}(\boldsymbol{\theta}, q) = \mathbb{E}_q \left[\log p(\mathbf{x}|\mathbf{z})\right] - \mathrm{D}_{\mathrm{KL}}(q \| p).$$

- The term "variational" is a historical accident: "variational inference" used to be done using variational calculus, but this isn't how we train VAEs.
- We'd like to choose q to make the bound as tight as possible.
- It's possible to show that the gap is given by:

$$\log p(\mathbf{x}) - \mathcal{F}(\boldsymbol{\theta}, q) = \mathrm{D}_{\mathrm{KL}}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x})).$$

Therefore, we'd like q to be as close as possible to the posterior distribution $p(\mathbf{z}|\mathbf{x})$.

- Let's think about the role of each of the two terms.
- The reconstruction term

$$\mathbb{E}_q[\log p(\mathbf{x}|\mathbf{z})] = -\frac{1}{2\sigma^2}\mathbb{E}_q[\|\mathbf{x} - G_{\boldsymbol{\theta}}(\mathbf{z})\|^2] + \mathrm{const}$$

  is minimized when q is a point mass on

$$\mathbf{z}_* = \arg\min_{\mathbf{z}} \|\mathbf{x} - G_{\boldsymbol{\theta}}(\mathbf{z})\|^2.$$

- But a point mass would have infinite KL divergence. (Exercise: check this.) So the KL term forces q to be more spread out.

Reparameterization Trick

- To fit q, let's assign it a parametric form, in particular a Gaussian distribution: $q(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$, where $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$ and $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_K^2)$.
- In general, it's hard to differentiate through an expectation. But for Gaussian q, we can apply the reparameterization trick:

$$z_i = \mu_i + \sigma_i \epsilon_i,$$

  where $\epsilon_i \sim \mathcal{N}(0, 1)$.
- Hence,

$$\overline{\mu_i} = \overline{z_i} \qquad \overline{\sigma_i} = \overline{z_i}\epsilon_i.$$

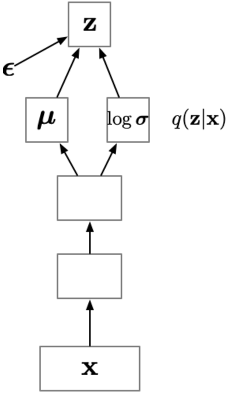
- This is exactly analogous to how we derived the backprop rules for droopout.

Amortization

- This suggests one strategy for learning the decoder. For each training example,
  1. Fit q to approximate the posterior for the current $\mathbf{x}$ by doing many steps of gradient ascent on $\mathcal{F}$.
  2. Update the decoder parameters $\boldsymbol{\theta}$ with gradient ascent on $\mathcal{F}$.
- **Problem:** this requires an expensive iterative procedure for every training example, so it will take a long time to process the whole training set.

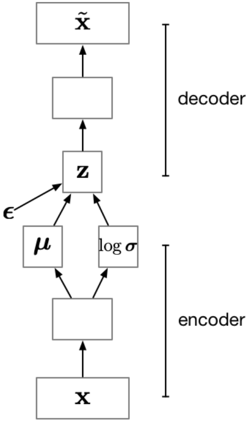
Amortization

- **Idea:** amortize the cost of inference by learning an inference network which predicts $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ as a function of $\mathbf{x}$.
- The outputs of the inference net are $\boldsymbol{\mu}$ and $\log \boldsymbol{\sigma}$. (The log representation ensures $\boldsymbol{\sigma} > 0$.)
- If $\boldsymbol{\sigma} \approx \mathbf{0}$, then this network essentially computes $\mathbf{z}$ deterministically, by way of $\boldsymbol{\mu}$.
  - But the KL term encourages $\boldsymbol{\sigma} > 0$, so in general $\mathbf{z}$ will be noisy.
- The notation $q(\mathbf{z}|\mathbf{x})$ emphasizes that q depends on $\mathbf{x}$, even though it's not actually a conditional distribution.



Amortization

- Combining this with the decoder network, we see the structure closely resembles an ordinary autoencoder. The inference net is like an encoder.
- Hence, this architecture is known as a variational autoencoder (VAE).
- The parameters of both the encoder and decoder networks are updated using a single pass of ordinary backprop.
  - The reconstruction term corresponds to squared error $\|\mathbf{x} - \tilde{\mathbf{x}}\|^2$, like in an ordinary VAE.
  - The KL term regularizes the representation by encouraging $\mathbf{z}$ to be more stochastic.

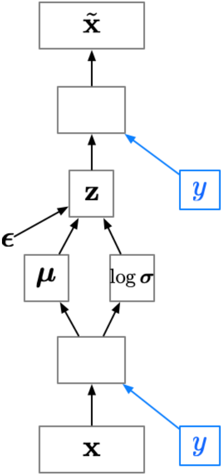


VAEs vs. Other Generative Models

- In short, a VAE is like an autoencoder, except that it's also a generative model (defines a distribution $p(\mathbf{x})$).
- Unlike autoregressive models, generation only requires one forward pass.
- Unlike reversible models, we can fit a low-dimensional latent representation. We'll see we can do interesting things with this...

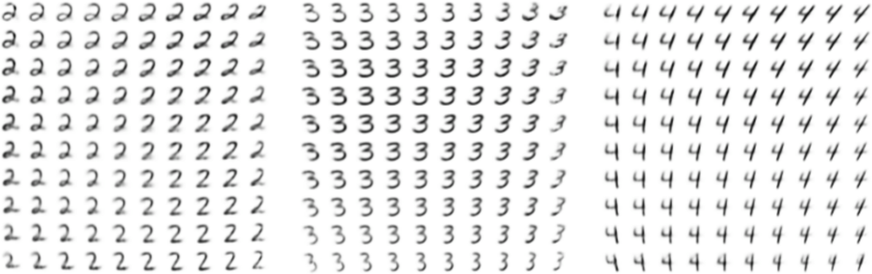
Class-Conditional VAE

- So far, we haven't used the labels y. A class-conditional VAE provides the labels to both the encoder and the decoder.
- Since the latent code $\mathbf{z}$ no longer has to model the image category, it can focus on modeling the stylistic features.
- If we're lucky, this lets us disentangle style and content. (Note: disentanglement is still a dark art.)
- See Kingma et al., "Semi-supervised learning with deep generative models."



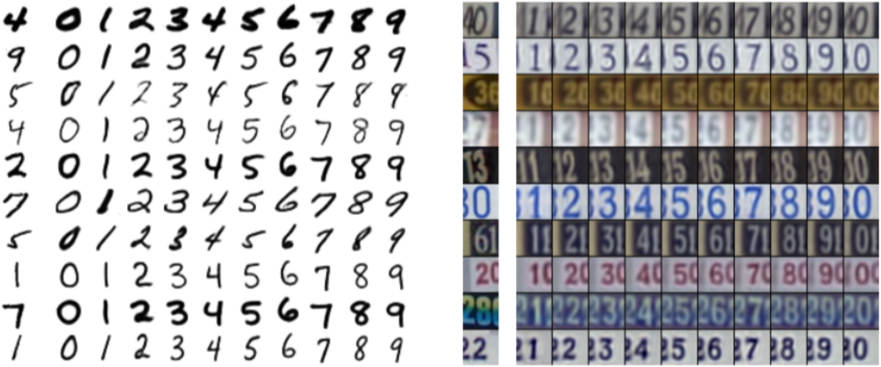
Class-Conditional VAE

- By varying two latent dimensions (i.e. dimensions of **z**) while holding y fixed, we can visualize the latent space.



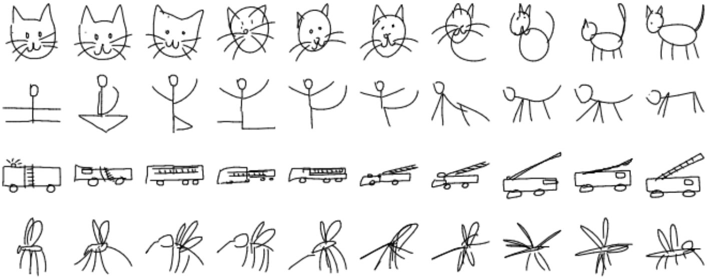
Class-Conditional VAE

- By varying the label y while holding $\mathbf{z}$ fixed, we can solve image analogies.



Latent Space Interpolations

- You can often get interesting results by interpolating between two vectors in the latent space:



Ha and Eck, "A neural representation of sketch drawings"

Latent Space Interpolations

- Latent space interpolation of music: `https://magenta.tensorflow.org/music-vae`