COMP9444: Neural Networks and Deep Learning

Week 9a. Autoencoders

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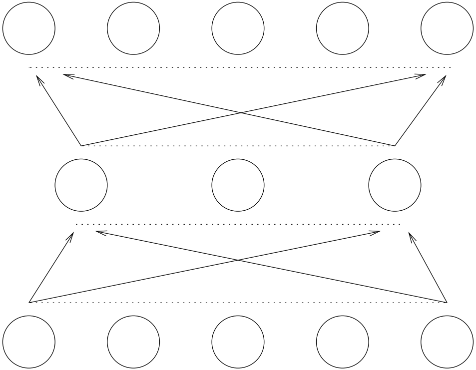
Outline

- Autoencoder Networks (14.1)
- Regularized Autoencoders (14.2)
- Stochastic Encoders and Decoders (14.4)
- Generative Models
- Variational Autoencoders (20.10.3)

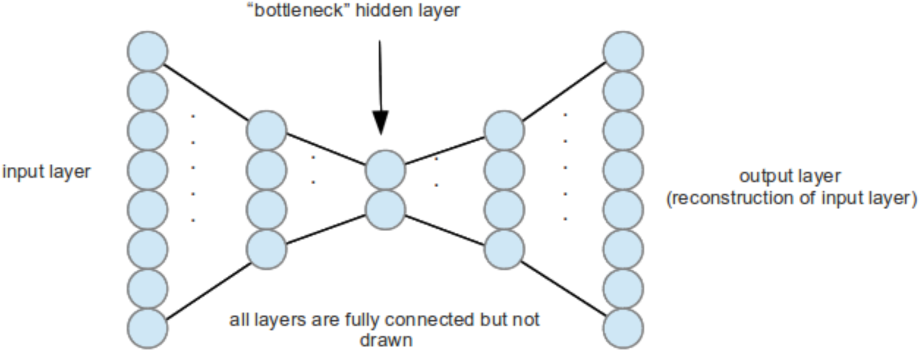
Recall: Encoder Networks



Inputs	Outputs
10000	10000
01000	01000
00100	00100
00010	00010
00001	00001

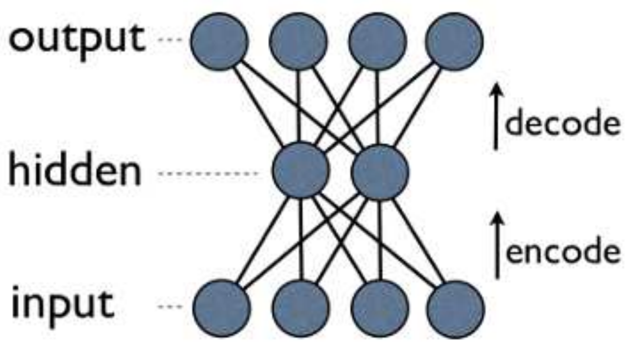
- identity mapping through a bottleneck
- also called N–M–N task
- used to investigate hidden unit representations

Autoencoder Networks



- ➣ output is trained to reproduce the input as closely as possible
- ➣ activations normally pass through a bottleneck, so the network is forced to compress the data in some way
- ➣ Autoencoders can be used to generate "fake" items, or to automatically extract abstract features from the input

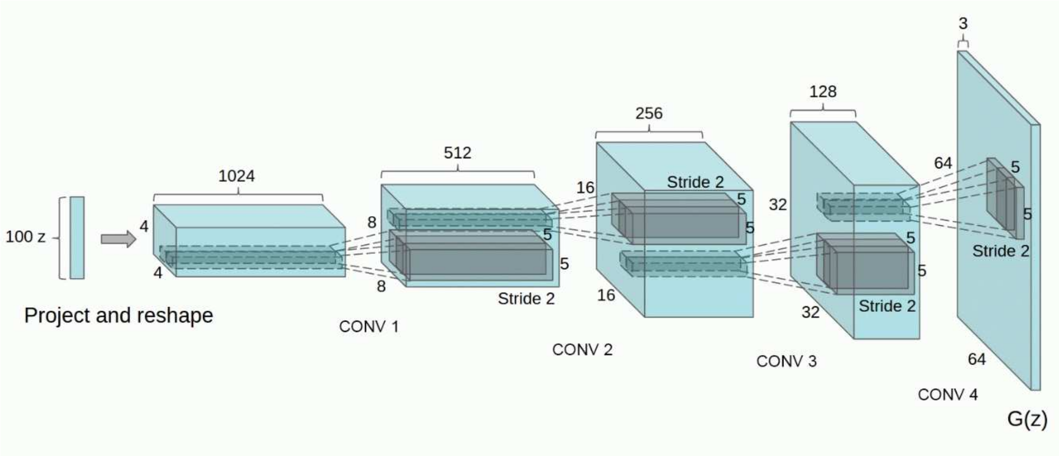
Autoencoder Networks



If the encoder computes $z = f(x)$ and the decoder computes $g(f(x))$ then we aim to minimize some distance function between x and $g(f(x))$

$$E = L\big(x, g(f(x))\big)$$

De-Convolutional Encoder for Images



Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks (Radford et al., 2016)

Autoencoder as Pretraining

- after an autoencoder is trained, the decoder part can be removed and replaced with, for example, a classification layer
- this new network can then be trained by backpropagaiton
- the features learned by the autoencoder then serve as initial weights for the supervised learning task

Regularized Autoencoders (14.2)

We may include additional loss term(s) in order to force the latent variables to conform to a certain distribution, or to achieve some other objective.

- Autoencoders with dropout at hidden layer(s)
- Sparse Autoencoders
- Contractive Autoencoders
- Denoising Autoencoders
- Variational Autoencoders
- Wasserstein Autoencoders

Sparse Autoencoder (14.2.1)

- One way to regularize an autoencoder is to include a penalty term in the loss function, based on the hidden unit activations.
- This is analagous to the weight decay term we previously used for supervised learning.
- One popular choice is to penalize the sum of the absolute values of the activations in the hidden layer

$$E = L(x, g(f(x))) + \lambda \sum_i |h_i|$$

- This is sometimes known as L_1-regularization (because it involves the absolute value rather than the square); it can encourage some of the hidden units to go to zero, thus producing a sparse representation.

Contractive Autoencoder (14.2.3)

- Another popular penalty term is the L_2-norm of the derivatives of the hidden units with respect to the inputs

$$E = L(x, g(f(x)) + \lambda \sum_i ||\nabla_x h_i||^2$$

- This forces the model to learn hidden features that do not change much when the training inputs x are slightly altered.

Denoising Autoencoder (14.2.2)

Another regularization method, similar to contractive autoencoder, is to add noise to the inputs, but train the network to recover the original input

repeat:

sample a training item $x^{(i)}$

generate a corrupted version $\tilde{x}$ *of* $x^{(i)}$

train to reduce $E = L\big(x^{(i)}, g(f(\tilde{x}))\big)$

end

Loss Functions and Probability

- We saw previously how the loss (cost) function at the output of a feedforward neural network (with parameters θ) can be seen as defining a probability distribution $p_\theta(x)$ over the outputs. We then train to maximize the log of the probability of the target values.
  - squared error assumes an underlying Gaussian distribution, whose mean is the output of the network
  - cross entropy assumes a Bernoulli distribution, with probability equal to the output of the network
  - softmax assumes a Boltzmann distribution

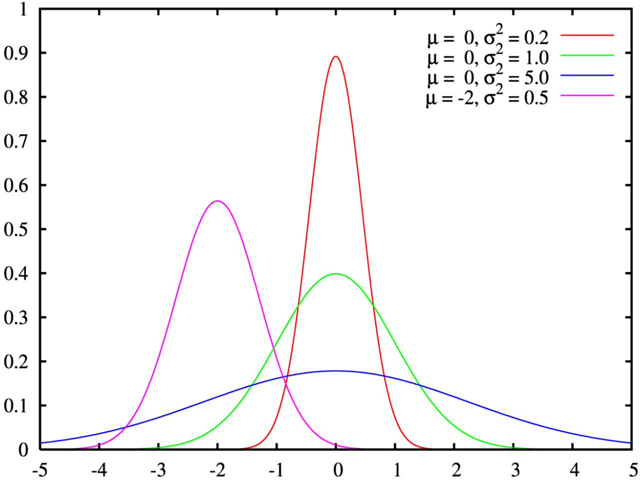
Stochastic Encoders and Decoders (14.4)

- For autoencoders, the decoder can be seen as defining a conditional probability distribution $p_\theta(x|z)$ of output x for a certain value z of the hidden or "latent" variables.
- In some cases, the encoder can also be seen as defining a conditional probability distribution $q_\phi(z|x)$ of latent variables z based on an input x .

Generative Models

- Sometimes, as well as reproducing the training items $\{x^{(i)}\}$, we also want to be able to use the decoder to generate new items which are of a similar "style" to the training items.
- In other words, we want to be able to choose latent variables z from a standard Normal distribution $p(z)$, feed these values of z to the decoder, and have it produce a new item x which is somehow similar to the training items.
- Generative models can be:
  - explicit (Variational Autoencoders, Wasserstein Autoencoders)
  - implicit (Generative Adversarial Networks)

Gaussian Distribution (3.9.3)



$\mu =$ mean

$\sigma =$ standard deviation

$$P_{\mu,\sigma}(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2/2\sigma^2}$$

Entropy and KL-Divergence

- The *entropy* of a distribution $q()$ is $$H(q) = \int_\theta q(\theta)(-\log q(\theta))d\theta$$
- In Information Theory, H(q) is the amount of information (bits) required to transmit a random sample from distribution $q()$
- For a Gaussian distribution, $$H(q) = \sum_i \log\, \sigma_i$$
- KL-Divergence $$\mathrm{D_{KL}}(q \,\|\, p) = \int_\theta q(\theta)(\log\, q(\theta) - \log\, p(\theta))d\theta$$
- $\mathrm{D_{KL}}(q \,\|\, p)$ is the number of *extra* bits we need to trasmit if we designed a code for $p()$ but the samples are drawn from $q()$ instead.
- If $p(z)$ is Standard Normal distribution, minimizing $D_{\mathrm{KL}}\big(q_\phi(z)\|p(z)\big)$ encourages $q_\phi()$ to center on zero and spread out to approximate $p()$.

KL-Divergence and Wasserstein Distance

Consider two Gaussian distributions q, p with mean μ_1, μ_2 and covariance Σ_1, Σ_2, respectively. In the case where $\mu_2 = 0$, $\Sigma_2 = \mathrm{I}$, the KL-Divergence between q and p simplifies to:

$$\mathrm{D}_{\mathrm{KL}}(q||p) = \frac{1}{2}\left[||\mu_1||^2 + \mathrm{Trace}(\Sigma_1) - \log|\Sigma_1| - d\right]$$

If $\Sigma_1 = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_d^2)$ is diagonal, this further simplifies to:

$$\mathrm{D}_{\mathrm{KL}}(q||p) = \frac{1}{2}\left[||\mu_1||^2 + \sum_{i=0}^{d}(\sigma_i^2 - 2\log(\sigma_i) - 1)\right]$$

which is minimized when $\mu_1 = 0$ and $\sigma_i = 1$ for all i .
The *Wasserstein Distance* between q and p is given by

$$W_2(q,p)^2 = ||\mu_1 - \mu_2||^2 + \mathrm{Trace}(\Sigma_1 + \Sigma_2 - 2(\Sigma_1\Sigma_2)^{\frac{1}{2}})$$

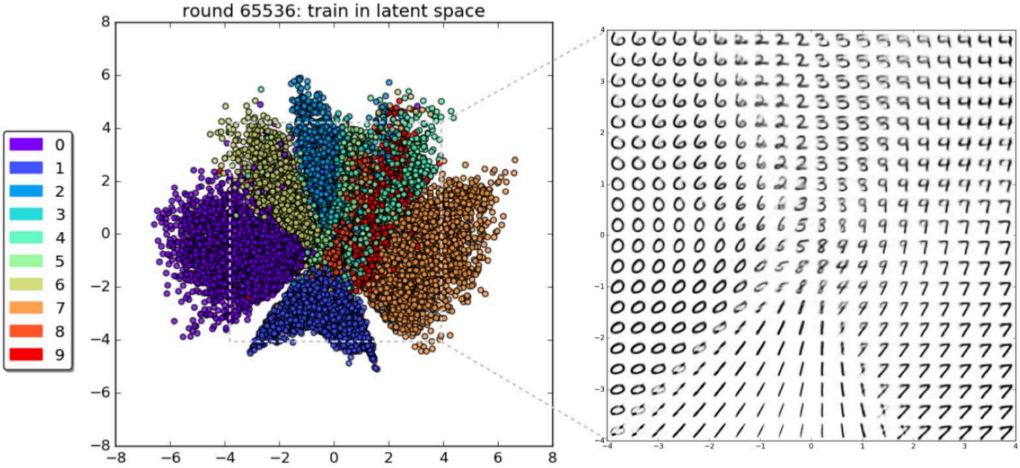
Variational Autoencoder (20.10.3)

Instead of producing a single z for each $x^{(i)}$, the encoder (with parameters ϕ) can be made to produce a mean $\mu_{z|x^{(i)}}$ and standard deviation $\sigma_{z|x^{(i)}}$
This defines a conditional (Gaussian) probability distribution $q_\phi(z|x^{(i)})$
We then train the system to maximize

$$\mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\big[\log\, p_\theta(x^{(i)}|z)\big] \;-\; D_{\mathrm{KL}}\big(q_\phi(z|x^{(i)})\|p(z)\big)$$

- the first term enforces that any sample z drawn from the conditional distribution $q_\phi(z|x^{(i)})$ should, when fed to the decoder, produce somthing approximating $x^{(i)}$
- the second term encourages $q_\phi(z|x^{(i)})$ to approximate $p(z)$
- in practice, the distributions $q_\phi(z|x^{(i)})$ for various $x^{(i)}$ will occupy complementary regions within the overall distribution $p(z)$

Variational Autoencoder Digits



Variational Autoencoder Digits

1st Epoch

9th Epoch

Original

Variational Autoencoder Faces

Variational Autoencoder

- Variational Autoencoder produces reasonable results
- tends to produce blurry images
- often end up using only a small number of the dimensions available to z

References

http://kvfrans.com/variational-autoencoders-explained/

http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture13.pdf

https://arxiv.org/pdf/1606.05908.pdf