### Outline



# COMP9444: Neural Networks and Deep Learning

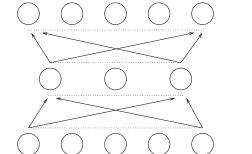
Week 9a. Autoencoders

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#### → Autoencoder Networks (14.1)

- → Regularized Autoencoders (14.2)
- → Stochastic Encoders and Decoders (14.4)
- ➤ Generative Models
- → Variational Autoencoders (20.10.3)

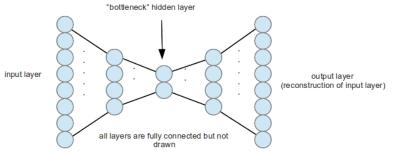
### **Recall: Encoder Networks**



InputsOutputs10000100000100001000001000010000010000100000100001

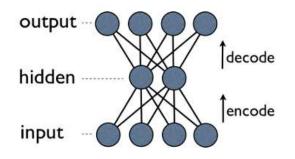
- ➤ identity mapping through a bottleneck
- ➤ also called N-M-N task
- → used to investigate hidden unit representations

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**

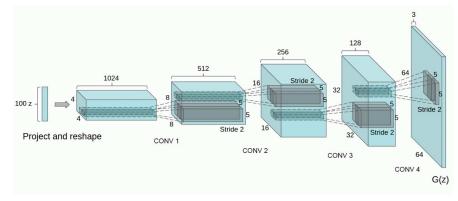


If the encoder computes z = f(x) and the decoder computes g(f(x)) then we aim to minimize some distance function between x and g(f(x))

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

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### **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<sub>1</sub>-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.

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#### **Contractive Autoencoder (14.2.3)**

➤ Another popular penalty term is the L<sub>2</sub>-norm of the derivatives of the hidden units with respect to the inputs

$$E = L(x, g(f(x)) + \lambda \sum_{i} ||\nabla_x h_i||^2$$

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

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## **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(x^{(i)}, g(f(\tilde{x})))
```

end

#### Loss Functions and Probability

- → We saw previously how the loss (cost) function at the output of a feedforward neural network (with parameters  $\theta$ ) 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

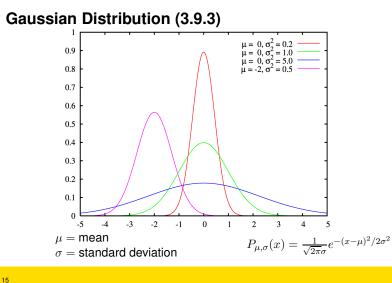
### **Stochastic Encoders and Decoders (14.4)**

- ➤ For autoencoders, the decoder can be seen as defining a conditional probability distribution p<sub>θ</sub>(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<sup>(i)</sup>}, 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)

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## **Entropy and KL-Divergence**

- → The *entropy* of a distribution q() is  $H(q) = \int_{a}^{b} q(\theta)(-\log q(\theta)) d\theta$
- → In Information Theory, H(q) is the amount of information (bits) required to transmit a random sample from distribution q()
- → For a Gaussian distribution,  $H(q) = \sum \log \sigma_i$
- → KL-Divergence  $D_{KL}(q || p) = \int_{\theta} q(\theta) (\log q(\theta) \log p(\theta)) d\theta$
- → D<sub>KL</sub>(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  $D_{\text{KL}}(q_{\phi}(z)||p(z))$ 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  $\mu_1, \mu_2$  and covariance  $\Sigma_1, \Sigma_2$ , respectively. In the case where  $\mu_2 = 0$ ,  $\Sigma_2 = I$ , the KL-Divergence between q and p simplifies to:

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

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

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

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

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

### Variational Autoencoder (20.10.3)

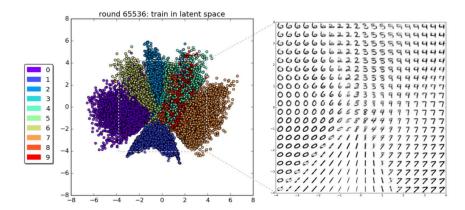
Instead of producing a single z for each  $x^{(i)}$ , the encoder (with parameters  $\phi$ ) can be made to produce a mean  $\mu_{z|x^{(i)}}$  and standard deviation  $\sigma_{z|x^{(i)}}$ . This defines a conditional (Gaussian) probability distribution  $q_{\phi}(z|x^{(i)})$ . We then train the system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

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

- → 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



19

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### Variational Autoencoder Faces



## Variational Autoencoder

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

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22

References

21

http://kvfrans.com/variational-autoencoders-explained/
http://cs231n.stanford.edu/slides/2017/cs231n\_2017\_lecture13.pdf
https://arxiv.org/pdf/1606.05908.pdf