Lecture 12: Autoencoders

CS109B Data Science 2
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I release a new SOTA which is not backwards-compatible with TF1.x / CUDA 9.

No problem. I upgrade my TensorFlow installation.

Fool! That's the second-oldest mistake, after Asian land wars: upgrading!

I train on CPU.
IT IS FRIDAY, ALL MY FRIENDS ARE AT PARTY

BUT, I'M HERE LEARNING BACK PROPAGATION
Announcements:

- Homework 3 deadline …
- Project group have been formed and will be announced …
“Pure” Reinforcement Learning (cherry)
- The machine predicts a scalar reward given once in a while.
- A few bits for some samples

Supervised Learning (icing)
- The machine predicts a category or a few numbers for each input
- Predicting human-supplied data
- 10→10,000 bits per sample

Unsupervised/Predictive Learning (cake)
- The machine predicts any part of its input for any observed part.
- Predicts future frames in videos
- Millions of bits per sample

(Yes, I know, this picture is slightly offensive to RL folks. But I’ll make it up)

Original LeCun cake analogy slide presented at NIPS 2016, the highlighted area has now been updated.
LeCun updated his cake recipe last week at the 2019 International Solid-State Circuits Conference (ISSCC) in San Francisco, replacing “unsupervised learning” with “self-supervised learning,” a variant of unsupervised learning where the data provides the supervision.
Outline

• What are autoencoders?
• Brief history of encoding/decoding.
• Inside autoencoders.
• Regularization of autoencoders.
• Applications
  • Denoising
  • Blending
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  • Blending
Quick Review. Neural Networks as function approximation.

Given an input $x$ and an output $y$ there exists a mapping from input space to output space as follows:

$$x \rightarrow y$$
$$y = f(x) + \epsilon$$

Our goal is to find an estimate of $f(x)$ which we will call $\hat{f}(x)$.

Statistical learning or modeling is the process of finding $\hat{f}(x)$.

Neural networks are one of many possible methods we can use to obtain the estimate $\hat{f}(x)$. 
Representational Learning

Representation Matters

\[ x \xrightarrow{\text{Linear Regression}} \hat{y} \]

- Fit quadratic function
- Do your best!

\[ y = x \]
Representational Learning

Representation Matters

\[ x_1, x_2 \rightarrow \text{Logistic Regression} \rightarrow \hat{y} \]

Fit polynomial function

Do your best!
Representational Learning

Representation Matters

\[ x \xrightarrow{\text{Learn Representation}} \phi(x) \xrightarrow{\text{Linear Regression}} \hat{y} \]

\[ \phi(x) = x^2 \]
Representational Learning

**Representation Matters**

\[ x \xrightarrow{\text{Learn Representation}} \phi(x) \xrightarrow{\text{Linear Regression}} \hat{y} \]

\[ r^2 = x_1^2 + x_2^2 \]
\[ \theta = \tan^{-1} \frac{x_2}{x_1} \]
Representational Learning

Representation Matters

\[ x \rightarrow \phi(x) \rightarrow \hat{y} \]
Representational Learning: **Supervised Learning**

We train the two networks by minimizing the loss function (cross entropy loss).

\[ \phi(x) \]

**Features**

\[ X \rightarrow \phi(x) \rightarrow Y \]

\{Cat, Dog\}

- Feature Discovery Network
- Classification Network
Representational Learning: **Self-supervised Learning**

We train the two networks by minimizing the cross entropy loss. 

\[ \text{Specialized features for Task} \]

\[ \phi(x) \]

\[ \{\text{Cat, Dog}\} \]
We train the two networks by minimizing the **reconstruction** loss function:

\[ L = \sum (x_i - \hat{x}_i)^2 \]

This is an **autoencoder**. It gets that name because it automatically finds the best way to encode the input so that the decoded version is as close as possible to the input.
Brief history of encoding/decoding

Is this a new idea?

- **MP3** can compress music files by a factor of 10 enabling digital storage and transmission of large volumes of audio.

- **JPG** compresses images by a factor of 10-20 and enables storage and transmission of image data.

- These technologies led the way to the image-rich web and abundance of music that we enjoy today.
We say that both MP3 and JPG take an input (a music or image file), and *encode* it into a *compressed* form.

Then we *decode* or *decompress* the intermediate version to some lower quality original version.
Lossless and Lossy Encoding

The greater the difference between the original version and the version post-decompression the greater the loss.

Example: Imagine you are in Boston and you want to write a birthday text to a special friend while walking home.

HANNAH HAPPY BIRTHDAY I LOVE YOU DAN

In the freezing Boston winter (-20C) you do not want to have your hands out in the open, so you shorten the message as much as possible using text-speak:

H HBD ILY D

Your 36 characters message is compressed to 11 characters
Lossless and Lossy Encoding (cont)

**Question:** Is this an example lossy or lossless compression?

*HPD* is unambiguous given that it is her birthday today, but *D* could mean *Dan* or *David* or *Donny* ... You can imagine the potential drama.

A way to test if a transformation is **lossy** or **lossless** is to consider if it can be inverted, or run backwards, to provide us with the original data. In autoencoders this is the loss function.
What are autoencoders?

- A particular kind of learning architecture.
- A mechanism of compressing inputs into a form that can later be decompressed similar to the way MP3 compresses audio and JPG compresses images.
- Autoencoders are more general than either MP3 or JPG.
- They are usually used to ...  
  - reduce data dimensionality or find a more general representation for many tasks
  - blend inputs from one input to another
  - denoising, infilling
  - ...
MP3 and JPG Image Compression

Original image 256x256=262,000, MP3=37,000, and JPG=26,000

Image taken from A. Glassner, Deep Learning, Vol. 2: From Basics to Practice
MP3 and JPG Image Compression (cont)

original  MP3  JPG

Image taken from A. Glassner, Deep Learning, Vol. 2: From Basics to Practice
The simplest autoencoder

Encode with a simple fully connected network (FCN)

- Image 100x100
- Flatten Image 10,000
- FCN with 20 neurons

Parameters: 10K x 20 + 20
The simplest autoencoder

Encode and decode together after training

- Image 100x100
- Flatten Image 10,000
- FCN with 20 neurons
- FCN with 10,000 neurons

Parameters: 10K x 20 + 20

Parameters: 10K x 20 + 10K

10,000 numbers

.reshape(100, 100)
Autoencoders in action

Comparing the input and output pixel by pixel.

Input Image 100x100  Output Image 100x100  Residuals 100x100
Bottleneck

- We start with 10,000 elements
- We have 20 in the middle
- And 10,000 elements again at the end
When you penalize your Natural Language Generation model for large sentence lengths

Me think, why waste time say lot word, when few word do trick.
Latent variables and latent layer

We say that an autoencoder is an example of semi-supervised or self-supervised learning.

It sort-of is supervised learning because we give the system explicit goal data (the output should be the same as the input), and it sort-of isn’t supervised learning because we don’t have any manually determined labels or targets on the inputs.
Autoencoders in action (cont)

Passing "Pavlos" to the trained autoencoder returns:

How about if we input the “Eagle”?
Autoencoders in action (cont)

We must **train** with a variety of images.
Autoencoders in action (cont)

After training with those images, let’s test how well it generalizes:

Network never seen anything like this, so it is no surprise that could not reconstruct this.
Autoencoders in action (cont)

We can use a better training set such as the Olivetti faces
A better autoencoder

MNIST data: train a simple AE with one-layer FCN encoder and one-layer FCN decoder
20 latent variables

<table>
<thead>
<tr>
<th>Original</th>
<th>Reconstructed</th>
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</thead>
<tbody>
<tr>
<td>72104</td>
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10 latent variables

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<tr>
<td>72104</td>
<td>72109</td>
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2 latent variables

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<th>Reconstructed</th>
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<tbody>
<tr>
<td>72104</td>
<td>93109</td>
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</table>

**WHY DOES IT WORK?**
For a better representation we can add neurons in one layer or go deeper.

28x28

Z is 20 dimensional

Original Images

Reconstructed Images

Deeper 20 latent variables
Shallow 20 latent variables

DEEPER IS BETTER
Exploring autoencoders

How can be sure that there is information in the latent space?

2 latent variables

original

reconstructed

20 neurons

10K neurons

How can be sure that there is information in the latent space?
Exploring autoencoders (cont)

For that let’s explore the actual latent space.

Input

```
7 2 1 0 4
```

Latent space

```
[Histograms of Z values]
```

Output

```
7 2 1 0 4
```
If latent space does not contain any information, then changing the values randomly won’t change the output or it will not be robust.

Input

Latent space

Output

Add random noise +/-10 to z’s
Exploring autoencoders (cont)

If latent space does not contain any information, then changing the values randomly won’t change the output or it will not be robust.

Input

Latent space

Output

Add random noise +/-100 to z’s
Exploring autoencoders (cont)

If latent space does not contain any information, then changing the values randomly won’t change the output or it will not be robust.

Input

Latent space

Add random noise +/-100 to z’s

Output
Exploring autoencoders (cont)

If latent space does not contain any information, then changing the values randomly won’t change the output or it will not be robust.

Input

Latent space

Output

Just noise
Further examine the latent space. Is there any separation of the different classes? If the AE learned the “essence” of the MNIST images, similar images should be close to each other.

Plot the latent space and examine the separation.

Here we plot the 2 PCA components of the latent space.
We blend inputs to create new data that is similar to the input data, but not exactly the same.

One example of blending is content blending where the content of two pieces of data is directly blended. An example is if we overlay images of a cow and zebra.
Blending

Content blending on MNIST images

Image taken from A. Glassner, Deep Learning, Vol. 2: From Basics to Practice
Another type of blending is **parametric** or **representation** blending:

In this type of blending we take advantage of parameterization to describe the objects we’re interested in. By engaging in blending in the parameter space, we can create results that blend the inherent qualities of the objects of interest.
Blending (cont)

Image taken from A. Glassner, Deep Learning, Vol. 2: From Basics to Practice
Parametric or representation blending

Image taken from A. Glassner, Deep Learning, Vol. 2: From Basics to Practice
Blending in compressed representation

While the blending we’ve described works well for uncompressed objects what happens when compression is involved?

The compressed form may not be the best representation with what we would like to blend the objects.

For example, let’s take the sounds of the words **cherry** and **orange**.

We can blend these sounds together or we can **compress them** into written words.
Blending Latent Variables

Back to the example of MNIST.

1. We start at the start of the arrows in latent space and then move to end of the arrow in 7 steps.
2. For each value of $z$ we use the already trained decoder to produce an image.

Image taken from A. Glassner, Deep Learning, Vol. 2: From Basics to Practice
Reconstructing Input Image
Applying to novel input

Check again if the deep AE trained on MNIST works with “Pavlos” image?

NO

Since we are dealing with images, it is best to use CNNs
Convolutional Autoencoders

28 x 28 x 1 → 16 x (3x3) ReLU
Output: 28 x 28 x 16

Max pooling 2x2
Output: 14 x 14 x 16

16 filters (3x3x1) same padding
Output: 28 x 28 x 16

2x2 → 8 x (3x3) ReLU
Output: 14 x 14 x 8

Max pooling 2x2
Output: 7 x 7 x 8

8 filters (3x3x16) same
Output: 14 x 14 x 8

3x (3x3) ReLU
2x2 → 16 x (3x3) ReLU
Output: 7 x 7 x 3

Max pooling 2x2
Output: 7 x 7 x 3

1 x (3x3) sigmoid
2x2 → 28 x 28 x 1
Convolutional Autoencoders

- 3 filters (3x3x8) same Output: 7x7x3
- Upsampling 2x2 Output: 14x14x3
- 16 filters (3x3x3) same Output: 14x14x16
- Upsampling 2x2 Output: 28x28x16
- 1 filter (3x3x16) same Output: 28x28x1

Nearest Neighbor

<table>
<thead>
<tr>
<th>Input: 2 x 2</th>
<th>Output: 4 x 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2</td>
<td>1 1 2 2</td>
</tr>
<tr>
<td>3 4</td>
<td>3 3 4 4</td>
</tr>
<tr>
<td>3 4</td>
<td>3 3 4 4</td>
</tr>
</tbody>
</table>
Convolutional Autoencoders

Original Images

Reconstructed Images with Conv AE

ConvAE latent variables
DeepFCN latent variables
Denoising

A popular use of autoencoders is to remove noise from samples.

Start with a **pristine** image.

Add noise to the input images.

Feed corrupted input into the autoencoder.

Measure reconstruction loss against **pristine** image.
Infilling

Claim is that AE learns the contextual information of the images. That would mean if some parts of the image is missing then

![Original - 0](image1.png) ![Mask - 0](image2.png) ![Recon - 0](image3.png)
Overcomplete Autoencoders

Over-complete autoencoder is when \( z \) has greater dimension than \( x \).

Autoencoder may simply copy input to output without learning anything useful – Mark’s point.

The ideal autoencoder model balances the following:

1. Sensitive to the inputs enough to accurately build a reconstruction.
2. Insensitive enough to the inputs that the model doesn't simply memorize or overfits the training data.
Overcomplete Autoencoders

• We’ve assumed so far that the size of the bottleneck is smaller than the size of the inputs – this is called an **undercomplete autoencoder**.
• The case in which the size of the bottleneck is greater than or equal to the number of inputs we call an **overcomplete autoencoder**.
Overcomplete Autoencoders

The size of the bottleneck (i.e. the number of latent variables) makes a difference!

<table>
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<tr>
<th>Latent Variables</th>
<th>Original</th>
<th>Reconstructed</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td><img src="72104.png" alt="Image" /></td>
<td><img src="72104.png" alt="Image" /></td>
</tr>
<tr>
<td>2</td>
<td><img src="72104.png" alt="Image" /></td>
<td><img src="92109.png" alt="Image" /></td>
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Regularized Autoencoders

- Sparse autoencoders
- Contractive autoencoders
- Denoising autoencoders and dropout
Sparse Autoencoders

This trade-off requires the model to maintain only the variations in the data required to reconstruct the input without holding on to redundancies within the input.

**Question:** How to achieve this?

For most cases, this involves constructing a loss function where one term encourages our model to be sensitive to the inputs (i.e. reconstruction loss $\mathcal{L}(x, \hat{x})$) and a second term discourages memorization/overfitting (i.e. an added regularizer).

$s(\cdot) = \log$
Sparse Autoencoders

- We allow our network to sensitize individual hidden layer nodes toward specific attributes of the input data.
- A sparse autoencoder is selectively activate regions of the network depending on the input data.
- Limiting the network's capacity to memorize the input data without limiting the networks capability to extract features from the data.

$\mathcal{L}(x, \hat{x}) + \lambda \sum_{i} |Z_i|$
Contractive Autoencoders

One would expect that for very similar inputs, the learned encoding would also be very similar.

We can explicitly train our model for this to be the case by requiring that the derivative of the hidden layer activations are small with respect to the input.

**Question:** How do we find how much the encoded space would change if the input changes?
Contractive Autoencoders

Derivatives

\[ \mathcal{L}(x, g(f(x))) + \lambda \sum_i ||\nabla_x z_i||^2 \]

This forces the model to learn a function that does not change much when \( x \) changes slightly. Because this penalty is applied only at training examples, it forces the autoencoder to learn features that capture information about the training distribution.
Denoising Autoencoders

The denoising autoencoder is an autoencoder that receives a corrupted data point as input and is trained to predict the original, uncorrupted data point as its output.

For each epoch:
Denoising autoencoders learn a manifold. Vector field learned by denoising autoencoder. Each arrow is proportional to \( g(f(x)) - x \).
Denoising Autoencoders (cont)

Vector field learned by denoising autoencoder. Each arrow is proportional to $g(f(x)) - x$
We allow our network to sensitize individual hidden layer nodes toward specific attributes of the input data.
Problems with Autoencoders

• Gaps in the latent space
• Separability in the latent space
• Discrete latent space