Neural Networks

Representations
Learning in the net

- Problem: Given a collection of input-output pairs, learn the function
• When the net must learn to classify..
  – Learn the classification boundaries that separate the training instances
• In reality
  – In general not really cleanly separated
    • So what is the function we learn?
In reality: Trivial linear example

- Two-dimensional example
  - Blue dots (on the floor) on the “red” side
  - Red dots (suspended at Y=1) on the “blue” side
  - No line will cleanly separate the two colors
Non-linearly separable data: 1-D example

- One-dimensional example for visualization
  - All (red) dots at Y=1 represent instances of class Y=1
  - All (blue) dots at Y=0 are from class Y=0
  - The data are not linearly separable
    - In this 1-D example, a linear separator is a threshold
    - No threshold will cleanly separate red and blue dots
Undesired Function

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What if?

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• What must the value of the function be at this X?
  – 1 because red dominates?
  – 0.9 : The average?
What if?

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  - 1 because red dominates?
  - 0.9: The average?

Estimate: \( P(1|X) \)

Potentially much more useful than a simple 1/0 decision
Also, potentially more realistic
What if?

• What must the value of the function be at this X?
  – 1 because red dominates?
  – 0.9: The average?

Estimate: $\approx P(1|X)$

Should an infinitesimal nudge of the red dot change the function estimate entirely?

If not, how do we estimate $P(1|X)$?
(since the positions of the red and blue X Values are different)

Potentially much more useful than a simple 1/0 decision
Also, potentially more realistic
The *probability* of $y=1$

- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the *probability* of $Y=1$ at that point
Consider this differently: at each point look at a small window around that point

Plot the average value within the window

- This is an approximation of the probability of 1 at that point
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This is an approximation of the probability of 1 at that point
The logistic regression model

\[ P(y=1|x) = \frac{1}{1 + e^{-(w_0 + w_1x)}} \]

- Class 1 becomes increasingly probable going left to right
  - Very typical in many problems
• A sigmoid perceptron with a single input models the *a posteriori* probability of the class given the input

\[
P(y|x) = \frac{1}{1 + e^{-(w_0 + w_1 x)}}
\]
Non-linearly separable data

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Logistic regression

\[ P(Y = 1|X) = \frac{1}{1 + \exp\left(-\left(\sum_i w_i x_i + w_0\right)\right)} \]

When \( X \) is a 2-D variable

- This the perceptron with a sigmoid activation
  - It actually computes the \textit{probability} that the input belongs to class 1
  - Decision boundaries may be obtained by comparing the probability to a threshold
    - These boundaries will be lines (hyperplanes in higher dimensions)
    - The sigmoid perceptron is a \textit{linear classifier}
Given the training data (many \((x, y)\) pairs represented by the dots), estimate \(w_0\) and \(w_1\) for the curve: 

\[
P(y|x) = f(x) = \frac{1}{1 + e^{-(w_0 + w_1x)}}
\]
Estimating the model

- Easier to represent using a $y = +1/-1$ notation

\[
P(y = 1|x) = \frac{1}{1+e^{-(w_0+w_1x)}}
\]

\[
P(y = -1|x) = \frac{1}{1+e^{(w_0+w_1x)}}
\]

\[
P(y|x) = \frac{1}{1+e^{-y(w_0+w_1x)}}
\]
Estimating the model

- Given: Training data $(X_1, y_1), (X_2, y_2), ..., (X_N, y_N)$
- $X$s are vectors, $y$s are binary (0/1) class values
- Total probability of data

$$P((X_1, y_1), (X_2, y_2), ..., (X_N, y_N)) = \prod_i P(X_i, y_i)$$

$$= \prod_i P(y_i|X_i) P(X_i) = \prod_i \frac{1}{1 + e^{-y_i(w_0 + w^T X_i)}} P(X_i)$$
Estimating the model

- Likelihood

\[
P(\text{Training data}) = \prod_i \frac{1}{1 + e^{-y_i(w_0 + w^T X_i)}} P(X_i)
\]

- Log likelihood

\[
\log P(\text{Training data}) = \sum_i \log P(X_i) - \sum_i \log \left( 1 + e^{-y_i(w_0 + w^T X_i)} \right)
\]
Maximum Likelihood Estimate

\[
\hat{w}_0, \hat{w}_1 = \arg\max_{w_0, w_1} \log P(\text{Training data})
\]

• Equals (note argmin rather than argmax)

\[
\hat{w}_0, \hat{w}_1 = \arg\min_{w_0, w} \sum_i \log \left( 1 + e^{-y_i(w_0 + w^T x_i)} \right)
\]

• Identical to minimizing the KL divergence between the desired output \( y \) and actual output

\[
\frac{1}{1 + e^{-(w_0 + w^T x_i)}}
\]

• Cannot be solved directly, needs gradient descent
So what about this one?

- Non-linear classifiers..
First consider the separable case..

• When the net must learn to classify..
First consider the separable case.

• For a “sufficient” net
First consider the separable case..

- For a “sufficient” net
- This final perceptron is a linear classifier
First consider the separable case..

• For a “sufficient” net
• This final perceptron is a linear classifier over the output of the penultimate layer
First consider the separable case.

• For perfect classification the output of the penultimate layer must be linearly separable
First consider the separable case..

- The rest of the network may be viewed as a transformation that transforms data from non-linear classes to linearly separable features.
First consider the separable case..

- The rest of the network may be viewed as a transformation that transforms data from non-linear classes to linearly separable features
  - We can now attach *any* linear classifier above it for perfect classification
  - Need not be a perceptron
  - Could even train an SVM on top of the features!
First consider the separable case.

- This is true of any sufficient structure
  - Not just the optimal one
- For insufficient structures, the network may attempt to transform the inputs to linearly separable features
  - Will fail to separate exactly, but will try to minimize error
Mathematically..

- \( y_{out} = \frac{1}{1+\exp(b+WTY)} = \frac{1}{1+\exp(b+WTf(X))} \)

- The data are (almost) linearly separable in the space of \( Y \)

- The network until the second-to-last layer is a non-linear function \( f(X) \) that converts the input space of \( X \) into the feature space \( Y \) where the classes are maximally linearly separable
A classification MLP actually comprises two components

- A “feature extraction network” that converts the inputs into linearly separable features
  - Or *nearly* linearly separable features
- A final linear classifier that operates on the linearly separable features
An SVM at the output?

• For binary problems, using an SVM with slack may be more effective than a final perceptron!
• How does that work??
  – Option 1: First train the MLP with a perceptron at the output, then detach the feature extraction, compute features, and train an SVM
  – Option 2: Directly employ a max-margin rule at the output, and optimize the entire network
  • Left as an exercise for the curious
How about the lower layers?

- How do the lower layers respond?
  - They too compute features
  - But how do they look

- Manifold hypothesis: For separable classes, the classes are linearly separable on a non-linear manifold

- Layers sequentially “straighten” the data manifold
  - Until the final layer, which fully linearizes it
The behavior of the layers

- Synthetic example: Feature space
The behavior of the layers

- CIFAR
The behavior of the layers

• CIFAR
When the data are not separable and boundaries are not linear.

- More typical setting for classification problems
Inseparable classes with an output logistic perceptron

- The “feature extraction” layer transforms the data such that the posterior probability may now be modelled by a logistic
Inseparable classes with an output logistic perceptron

- The “feature extraction” layer transforms the data such that the posterior probability may now be modelled by a logistic
  - The output logistic computes the posterior probability of the class given the input

\[ P(y|x) = f(x) = \frac{1}{1 + e^{-(w_0 + w^T x)}} \]
When the data are not separable and boundaries are not linear.

- The output of the network is $P(y|x)$
  - For multi-class networks, it will be the *vector* of a posteriori class probabilities
Everything in this book may be wrong!

- Richard Bach (Illusions)
There’s no such thing as inseparable classes

- A sufficiently detailed architecture can separate nearly *any* arrangement of points
  - “Correctness” of the suggested intuitions subject to various parameters, such as regularization, detail of network, training paradigm, convergence etc..
Changing gears..
Intermediate layers

We’ve seen what the network learns here

But what about here?
Recall: The basic perceptron

• What do the weights tell us?
  – The neuron fires if the inner product between the weights and the inputs exceeds a threshold

\[
y = \begin{cases} 
1 & \text{if } \sum_i w_i x_i \geq T \\
0 & \text{else}
\end{cases}
\]

\[
y = \begin{cases} 
1 & \text{if } x^T w \geq T \\
0 & \text{else}
\end{cases}
\]
Recall: The weight as a “template”

- The perceptron fires if the input is within a specified angle of the weight
  - Represents a convex region on the surface of the sphere!
  - The network is a Boolean function over these regions.
    - The overall decision region can be arbitrarily nonconvex
- Neuron fires if the input vector is close enough to the weight vector.
  - If the input pattern matches the weight pattern closely enough
Recall: The weight as a template

• If the correlation between the weight pattern and the inputs exceeds a threshold, fire
• The perceptron is a correlation filter!

\[
y = \begin{cases} 
1 & \text{if } \sum_i w_i x_i \geq T \\
0 & \text{else} 
\end{cases}
\]
The lowest layers of a network detect significant features in the signal
  – The neurons are correlation filters for these features

The more features we detect, the more information we retain about the input
• The higher level layers detect patterns of patterns
  – E.g. neurons in the second layer of this net may detect digits
    • Fire if the pattern of first-layer patterns form the digit
  – The topmost layer is just a single neuron that would detect if *any* of the second-layer neurons fired
Recall: MLP features

- The lowest layers of a network detect significant features in the signal
- The signal could be (partially) reconstructed using these features
  - Will retain all the significant components of the signal
Making it explicit

• The signal could be (partially) reconstructed using these features
  – Will retain all the significant components of the signal

• Simply *recompose* the detected features
  – Will this work?
Making it explicit

• The signal could be (partially) reconstructed using these features
  – Will retain all the significant components of the signal
• Simply *recompose* the detected features
  – Will this work?

Not in this problem.
The network is optimized to recognize digits
Will only retain distinctly digit-like or obviously not-digit like features
Rest are irrelevant and will be lost
Making it explicit: an autoencoder

- A neural network can be trained to predict the input itself
- This is an autoencoder
- An encoder learns to detect all the most significant patterns in the signals
- A decoder recomposes the signal from the patterns
The Simplest Autencoder

- A single hidden unit
- Hidden unit has linear activation
- What will this learn?
The Simplest Autencoder

Training: Learning $\mathcal{W}$ by minimizing L2 divergence

$$\hat{x} = w^T wx$$
$$div(\hat{x}, x) = \|x - \hat{x}\|^2 = \|x - w^T wx\|^2$$

$$\hat{\mathcal{W}} = \arg\min_{\mathcal{W}} E[div(\hat{x}, x)]$$
$$\hat{\mathcal{W}} = \arg\min_{\mathcal{W}} E[\|x - w^T wx\|^2]$$

• This is just PCA!
The Simplest Autencoder

- The autoencoder finds the direction of maximum energy
  - Variance if the input is a zero-mean RV
- All input vectors are mapped onto a point on the principal axis
The Simplest Autencoder

• Simply varying the hidden representation will result in an output that lies along the major axis
The Simplest Autencoder

- Simply varying the hidden representation will result in an output that lies along the major axis.
- This will happen even if the learned output weight is separate from the input weight.
  - The minimum-error direction is the principal eigen vector.
For more detailed AEs without a non-linearity

\[ \hat{X} = W^T Y \]

\[ Y = WX \]

\[ E = \|X - W^T WX\|^2 \]

Find \( W \) to minimize \( \text{Avg}[E] \)

- This is still just PCA
  - The output of the hidden layer will be in the principal subspace
  - Even if the recomposition weights are different from the “analysis” weights
Terminology:

- **Encoder**: The “Analysis” net which computes the hidden representation

- **Decoder**: The “Synthesis” which recomposes the data from the hidden representation
Introducing nonlinearity

- When the hidden layer has a *linear* activation the decoder represents the best *linear* manifold to fit the data
  - Varying the hidden value will move along this linear manifold
- **When the hidden layer has non-linear activation, the net performs nonlinear PCA**
  - The decoder represents the best non-linear manifold to fit the data
  - Varying the hidden value will move along this non-linear manifold
The AE

- With non-linearity
  - "Non linear" PCA
  - Deeper networks can capture more complicated manifolds
    - "Deep" autoencoders
Some examples

- 2-D input
- Encoder and decoder have 2 hidden layers of 100 neurons, but hidden representation is unidimensional
- Extending the hidden “z” value beyond the values seen in training does not continue along a helix
Some examples

• The model is specific to the training data..
  – Varying the hidden layer value only generates data along the learned manifold
    • *Any input* will result in an output along the learned manifold
  – But may not generalize beyond the manifold
When the hidden representation is of lower dimensionality than the input, often called a “bottleneck” network

- Nonlinear PCA
- Learns the manifold for the data
  - If properly trained
The AE

- The decoder can only generate data on the manifold that the training data lie on.
- This also makes it an excellent “generator” of the distribution of the training data.
  - Any values applied to the (hidden) input to the decoder will produce data similar to the training data.
The Decoder:

- The decoder represents a source-specific generative dictionary
- Exciting it will produce typical data from the source!
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A cute application..

• Signal separation...

• Given a mixed sound from multiple sources, separate out the sources
Dictionary-based techniques

• Basic idea: Learn a dictionary of “building blocks” for each sound source
• All signals by the source are composed from entries from the dictionary for the source
Dictionary-based techniques

- Learn a similar dictionary for all sources expected in the signal
Dictionary-based techniques

- A mixed signal is the linear combination of signals from the individual sources
  - Which are in turn composed of entries from its dictionary
Dictionary-based techniques

• Separation: Identify the combination of entries from both dictionaries that compose the mixed signal
Dictionary-based techniques

- **Separation**: Identify the combination of entries from both dictionaries that compose the mixed signal
  - The composition from the identified dictionary entries gives you the separated signals
Learning Dictionaries

• Autoencoder dictionaries for each source
  – Operating on (magnitude) spectrograms

• For a well-trained network, the “decoder” dictionary is highly specialized to creating sounds for that source
Model for mixed signal

Estimate $I_1()$ and $I_2()$ to minimize cost function $J()$

- The sum of the outputs of both neural dictionaries
  - For some unknown input
Separation

Test Process

Given mixed signal and source dictionaries, find excitation that best recreates mixed signal

- Simple backpropagation

Intermediate results are separated signals

Cost function

\[ J = \sum ||X(f, t) - Y(f, t)||^2 \]

Estimate \( I_1 \) and \( I_2 \) to minimize cost function \( J() \)

- Given mixed signal and source dictionaries, find excitation that best recreates mixed signal
  - Simple backpropagation

Intermediate results are separated signals
Example Results

5-layer dictionary, 600 units wide

• Separating music
Story for the day

• Classification networks learn to predict the *a posteriori* probabilities of classes
  – The network until the final layer is a feature extractor that converts the input data to be (almost) linearly separable
  – The final layer is a classifier/predictor that operates on linearly separable data

• Neural networks can be used to perform linear or non-linear PCA
  – "Autoencoders"
  – Can also be used to compose constructive dictionaries for data
    • Which, in turn can be used to model data distributions