Introduction to Deep Neural Networks (1)

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Introduction to Machine Learning (CS771A)

October 23, 2018
Linear Models (and their limitations..)

- Linear models: Output produced by taking a linear combination of input features

\[ y_n = \sum_{d=1}^{D} w_d x_{nd} \]

Some monotonic function (e.g., sigmoid)

- Already seen several examples (linear regression, logistic regression, linear SVM, multi-output linear regression, softmax regression, and several others)

- This basic architecture is classically also known as the "Perceptron" (not to be confused with the Perceptron "algorithm", which learns a linear classification model)

- This simple model can’t however learn complex functions (e.g., nonlinear decision boundaries)

- We have already seen a way of handling nonlinearities: Kernel Methods (invented in the 90s)

- Something existed in the pre-kernel methods era, too..
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Neural Networks a.k.a. Multi-layer Perceptron (MLP)

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Mathematical formulations:
- Output layer: $y_n = o \left( \sum_{k=1}^{K} v_k h_{nk} \right)$
- Hidden layer: $h_{nk} = g \left( \sum_{d=1}^{D} w_{dk} x_{nd} \right)$
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Each node (a.k.a. unit) in the hidden layer computes a nonlinear transform of inputs it receives
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- The overall effect is a nonlinear mapping from inputs to outputs (justification later)
Illustration: A Neural Network with One Hidden Layer

Each input $x_n$ transformed into several “pre-activations” using linear models:

$$a_{nk} = w_k^\top x_n = D \sum_{d=1}^D w_{dk} x_{nd}$$

Nonlinear activation applied on each pre-activation:

$$h_{nk} = g(a_{nk})$$

A linear model applied on the new “features”:

$$s_n = v_k^\top h_{nk} = K \sum_{k=1}^K v_k h_{nk}$$

Finally, the output is produced as:

$$y_n = o(s_n)$$

Unknowns of the model ($w_1, \ldots, w_K$ and $v$) learned by minimizing a loss $L(W, v) = \sum_{n=1}^N \ell(y_n, o(s_n))$, e.g., squared, logistic, softmax, etc (depending on the output).
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Unknowns of the model (\( w_1, \ldots, w_K \) and \( v \)) learned by minimizing a loss

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- Each input $x_n$ transformed into several “pre-activations” using linear models
  
  $$a_{nk} = w_k^T x_n = \sum_{d=1}^{D} w_{dk} x_{nd}$$

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Can even be identity (e.g., for regression $y_n = s_n$)
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Neural Networks: A Basic Pictorial Representation

- Note: Hidden layer pre-activations $a_{nk}$ and post-activations $h_{nk}$ will be shown together for brevity.

Single Hidden Layer

More succintly..
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We will only show $h_{nk}$ to denote the value computed by the $k$-th hidden unit.
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More succintly.. Single Hidden Layer

- We will only show $h_{nk}$ to denote the value computed by the $k$-th hidden unit.
- Likewise, for the output layer, we will directly show the final output $y_n$. 

$y_n = o \left( \sum_{k=1}^{K} v_k h_{nk} \right)$

$y_n = o \left( \sum_{d=1}^{P} w_{dk} x_{nd} \right)$
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More succintly...

- We will only show $h_{nk}$ to denote the value computed by the $k$-th hidden unit
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- Each node in hidden/output layers computes a linear trans. of its inputs + applies a nonlinearity
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Likewise, for the output layer, we will directly show the final output $y_n$.
Each node in hidden/output layers computes a linear trans. of its inputs + applies a nonlinearity.
Different layers can use different types of activations (output layer may have none).
MLPs Can Learn Nonlinear Functions: A Justification

- An MLP can be seen as a **composition of multiple linear models** combined non-linearly
- Let's look at a simple example of 2-dim inputs that are linearly not separable

A Multi-layer Perceptron Classifier (one hidden layer with 2 units) Capable of learning nonlinear boundaries

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Standard Single "Perceptron" Classifier (no hidden units) Cannot learn nonlinear boundaries

MLP with a single, sufficiently wide hidden layer can approximate any function (Hornick, 1991)
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![Diagram](image)

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\[ y_n = \sum w_i x_i \]

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Examples of some NN/MLP architectures
Neural Networks with One Hidden Layer

- Already saw the special case of a single layer NN ($D = 3$, $K = 2$)

$W = [w_1, \ldots, w_K]$, with $w_k$ being the weights incident on $k$-th hidden unit

- Each $w_k$ acts as a "feature detector" or "filter" (and there are $K$ such filters in the above NN)
Neural Networks with One Hidden Layer

- Already saw the special case of a single layer NN \((D = 3, \ K = 2)\)
- In general, an NN with \(D\) input units and a single hidden layer with \(K\) units

\[
W = \begin{bmatrix}
w_{11} & \cdots & w_{1K} \\
\vdots & \ddots & \vdots \\
w_{D1} & \cdots & w_{DK}
\end{bmatrix}
\]

\[
v = \begin{bmatrix} v_1 \\
\vdots \\
v_K
\end{bmatrix}
\]

\[
h_n = g(W^\top x_n)
\]

\[
y_n = o(v^\top h_n)
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Note: \(w_{dk}\) is the weight of edge between input layer node \(d\) and hidden layer node \(k\)
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\[
\begin{align*}
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Neural Networks with One Hidden Layer and Multiple Outputs

- Very common in multi-class or multi-output/multi-label learning problems
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- An NN with $D$ input units, single hidden layers with $K$ units, and multiple outputs

\[ y_n = o(V^\top h_n) \]

\[ h_n = g(W^\top x_n) \]

\[ v = \begin{bmatrix} v_{11} & \cdots & v_{1C} \\ \vdots & \ddots & \vdots \\ v_{K1} & \cdots & v_{KC} \end{bmatrix} \]

\[ w = \begin{bmatrix} w_{11} & \cdots & w_{1K} \\ \vdots & \ddots & \vdots \\ w_{D1} & \cdots & w_{DK} \end{bmatrix} \]
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$$h_n = g(W^T x_n)$$

$$w = \begin{bmatrix} w_{11} & \cdots & w_{1K} \\ \vdots & \ddots & \vdots \\ w_{D1} & \cdots & w_{DK} \end{bmatrix}$$

- Similar to multi-output regression or softmax regression on $h_n$ as features
An NN with $D$ input units, multiple hidden layers, and multiple outputs

- Hidden Layer 1
- Hidden Layer 2
- Hidden Layer L

Note: This (and also the previous simpler ones) is called a fully-connected feedforward network

- Fully connected: All pairs of units between adjacent layers are connected to each other
- Feedforward: No backward connections. Also, only nodes in adjacent layers connected

$y_{n1} \quad y_{n2} \quad \ldots \quad y_{nC}$

$V$ is $K_L \times C$

$K_L$ hidden units

$W^{(l)}$ is $K_{l-1} \times K_l$ ($l = 1, \ldots, L$ and $K_0 = D$)

$y_{n1} \quad y_{n2} \quad \ldots \quad y_{nK_1}$

$K_1$ hidden units

$W^{(1)}$ is $D \times K_1$

$x_{n1} \quad x_{n2} \quad \ldots \quad x_{nD}$

$D$ visible units
Neural Networks: Multiple Hidden Layers and Multiple Outputs

- An NN with $D$ input units, multiple hidden layers, and multiple outputs

![Neural Network Diagram]

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Neural Networks are Feature Learners!

- An NN (single/multiple hidden layers) tries to learn features that can predict the output well.

A learned mapping, unlike kernel methods where the mapping was pre-defined by the choice of kernel.
Deep neural networks are good at detecting features at multiple layers of abstraction. The connection weights between layers can be thought of as feature detectors or “filters.”

- $K_1 = 100$
- $K_2 = 32$
- $K_3 = 24$

Low-level feature detectors (e.g., detect edges)

Higher-level feature detectors (e.g., parts of face)

Even higher-level feature detectors (make classification easy)
Deep neural networks are good at detecting features at multiple layers of abstraction.

The connection weights between layers can be thought of as feature detectors or “filters”.

Lowest layer weights detect generic features, higher level weights detect more specific features.
Deep neural networks are good at detecting features at **multiple layers of abstraction**

The **connection weights** between layers can be thought of as **feature detectors or “filters”**

- Lowest layer weights detect **generic features**, higher level weights detect more **specific features**
- Features learned in one layer are composed of features learned in the layer below
Why Are Neural Network Learned Features Helpful?

A single layer model will learn an "average" feature detector. Can't capture subtle variations in the inputs. An MLP can learn multiple feature detectors (even with a single hidden layer). Therefore even a single hidden layer helps capture subtle variations in the inputs.
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\[ y_n = \sum h_n w \]

\[ h_n = \sum x_n w \]

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Learning Neural Networks via Backpropagation

- Backpropagation = Gradient descent using chain rule of derivatives

The chain rule of derivatives states: if $y = f_1(x)$ and $x = f_2(z)$ then $\frac{\partial y}{\partial z} = \frac{\partial y}{\partial x} \cdot \frac{\partial x}{\partial z}$.

Since neural networks have a "recursive" architecture, backprop is especially useful.

Basic idea: Start taking the derivatives from output layer and proceed backwards (hence the name).

Using backprop in neural nets enables us to reuse previous computations efficiently.
Learning Neural Networks via Backpropagation

- Backpropagation = Gradient descent using chain rule of derivatives
- (Current) Ideal way for learning deep neural networks

Chain rule of derivatives: Example, if $y = f_1(x)$ and $x = f_2(z)$ then $\frac{\partial y}{\partial z} = \frac{\partial y}{\partial x} \frac{\partial x}{\partial z}$

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![Diagram of a neural network](image)

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Basic idea: Start taking the derivatives from output layer and proceed **backwards** (hence the name)

Using backprop in neural nets enables us to **reuse previous computations** efficiently
Learning Neural Networks via Backpropagation

- Backprop iterates between a forward pass and a backward pass

Implementing backprop by hand may be very cumbersome for complex, very deep NNs.

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Activation Functions

- Some common activation functions

- Sigmoid: $h = \sigma(a) = \frac{1}{1 + \exp(-a)}$

- Tanh (tan hyperbolic): $h = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} = 2\sigma(2a) - 1$

- ReLU (Rectified Linear Unit): $h = \max(0, a)$

- Leaky ReLU: $h = \max(\beta a, a)$ where $\beta$ is a small positive number

Several others, e.g., Softplus $h = \log(1 + \exp(a))$, exponential ReLU, maxout, etc.

Sigmoid, tanh can have issues during backprop (saturating gradients, non-centered)

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  - Complex network (several, very wide hidden layers) or simple network (few, moderately wide hidden layers)?
  - Aren’t deep neural network prone to overfitting (since they contain a huge number of parameters)?
Representational Power of Hidden Layers

- Consider an NN with a single hidden layer
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Recall that each hidden unit “adds” a function to the overall function

Very large $K$ seems to overfit. Should we instead prefer small $K$? No! It is better to use large $K$ and regularize well. Here is a reason/justification:

Simple NN with small $K$ will have a few local optima, some of which may be bad.

Complex NN with large $K$ will have many local optima, all equally good.

Note: The above interesting behavior of NN has some theoretical justifications (won’t discuss here)

We can also use multiple hidden layers (each sufficiently large) and regularize well.
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![Diagram of a neural network with a single hidden layer](image.png)

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(Preventing) Overfitting in Neural Networks

- Complex single/multiple hidden layer NN can overfit

- Many ways to avoid overfitting, such as
  - Standard regularization on the weights, such as $\ell_2$, $\ell_1$, etc. ($\ell_2$ reg. is also called weight decay)

- Single Hidden Layer NN with $K = 20$ hidden units and L2 regularization

- Early stopping (traditionally used): Stop when validation error starts increasing

- Dropout: Randomly remove units (with some probability $p \in (0, 1)$) during training

---

Input Layer

Hidden Layer 1

Hidden Layer 1

Hidden Layer 2

Output Layer
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Wide or Deep?

- While very wide single hidden layer can approx. any function, often we prefer many hidden layers

\[
\begin{align*}
K_1 &= 100 \\
K_2 &= 32 \\
K_3 &= 24 \\
\end{align*}
\]

- Lower-level feature detectors (e.g., detect edges)
- Higher-level feature detectors (e.g., parts of face)
- Even higher-level feature detectors (make classification easy)

- Higher layers help learn more directly useful/interpretable features (also useful for compressing data using a small number of features)
Kernel Methods vs Deep Neural Nets

- Recall the prediction rule for a kernel method (e.g., kernel SVM)

\[ y = \sum_{n=1}^{N} \alpha_n k(x_n, x) \]

This is analogous to a single hidden layer NN with fixed/pre-defined hidden nodes \( \{k(x_n, x)\}_{n=1}^{N} \) and output layer weights \( \{\alpha_n\}_{n=1}^{N} \).

The prediction rule for a deep neural network

\[ y = K \sum_{k=1}^{V} v_k h_k \]

Here, the \( h_k \)'s are learned from data (possibly after multiple layers of nonlinear transformations).

Both kernel methods and deep NNs be seen as using nonlinear basis functions for making predictions. Kernel methods use fixed basis functions (defined by the kernel) whereas NN learns the basis functions adaptively from data.
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Deep Neural Nets for Unsupervised Learning

- Can use neural nets for dimensionality reduction
- A popular approach is to use autoencoders
- Autoencoder: Compress the input and uncompress to reconstruct
- An encoder (a neural net) does compression and a decoder (a neural net) does decompression

In an NN based autoencoder, the output layer is the same as the input!
Deep Neural Nets: Some Comments

- Highly effective in learning good feature representations from data in an “end-to-end” manner
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- Deep learning models can also be probabilistic and generative (will look at some of it in next class)
Other types of deep neural networks, e.g.,

- Convolutional Neural Networks (especially suited for images); not “fully connected”

- Neural networks for sequence data (e.g., text)

- Some optimization methods especially popular for neural networks

- An overview of other recent advances in deep learning