## CS 188: Artificial Intelligence Neural Networks



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(Slides adapted from Pieter Abbeel, Dan Klein, Anca Dragan, Stuart Russell and Dawn Song)

## Separable Case: Probabilistic Decision - Clear Preference




## Best w?

- Maximum likelihood estimation:

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

with:

$$
\begin{aligned}
& P\left(y^{(i)}=+1 \mid x^{(i)} ; w\right)=\frac{1}{1+e^{-w \cdot f\left(x^{(i)}\right)}} \\
& P\left(y^{(i)}=-1 \mid x^{(i)} ; w\right)=1-\frac{1}{1+e^{-w \cdot f\left(x^{(i)}\right)}}
\end{aligned}
$$

= Logistic Regression

## Multiclass Logistic Regression

- Recall Perceptron:
- A weight vector for each class: $w_{y}$
- Score (activation) of a class y: $w_{y} \cdot f(x)$
- Prediction highest score wins $y=\arg \underset{y}{\max } w_{y} \cdot f(x)$

- How to make the scores into probabilities?

original activations
softmax activations


## Best w?

- Maximum likelihood estimation:

$$
\begin{gathered}
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right) \\
P\left(y^{(i)} \mid x^{(i)} ; w\right)=\frac{e^{w_{y}(i) \cdot f\left(x^{(i)}\right)}}{\sum_{y} e^{w_{y} \cdot f\left(x^{(i)}\right)}}
\end{gathered}
$$

## Optimization

## Optimization

i.e., how do we solve:

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

## Hill Climbing

Recall from CSPs lecture: simple, general idea Start wherever Repeat: move to the best neighboring state If no neighbors better than current, quit


What's particularly tricky when hill-climbing for multiclass logistic regression?

- Optimization over a continuous space
- Infinitely many neighbors!
- How to do this efficiently?


## 1-D Optimization



Could evaluate $g\left(w_{0}+h\right)$ and $g\left(w_{0}-h\right)$
Then step in best direction
Or, evaluate derivative: $\frac{\partial g\left(w_{0}\right)}{\partial w}=\lim _{h \rightarrow 0} \frac{g\left(w_{0}+h\right)-g\left(w_{0}-h\right)}{2 h}$
Tells which direction to step into

## 2-D Optimization



## Gradient Ascent

Perform update in uphill direction for each coordinate The steeper the slope (i.e. the higher the derivative) the bigger the step for that coordinate
E.g., consider: $g\left(w_{1}, w_{2}\right)$

Updates:

$$
\begin{aligned}
& w_{1} \leftarrow w_{1}+\alpha * \frac{\partial g}{\partial w_{1}}\left(w_{1}, w_{2}\right) \\
& w_{2} \leftarrow w_{2}+\alpha * \frac{\partial g}{\partial w_{2}}\left(w_{1}, w_{2}\right)
\end{aligned}
$$

- Updates in vector notation:

$$
w \leftarrow w+\alpha * \nabla_{w} g(w)
$$

with: $\nabla_{w} g(w)=\left[\begin{array}{l}\frac{\partial g}{\partial w_{1}}(w) \\ \frac{\partial g}{\partial w_{2}}(w)\end{array}\right] \quad=$ gradient

## Gradient Ascent

Idea:
Start somewhere
Repeat: Take a step in the gradient direction


## Gradient in n dimensions

$$
\nabla g=\left[\begin{array}{c}
\frac{\partial g}{\partial w_{1}} \\
\frac{\partial g}{\partial w_{2}} \\
\cdots \\
\frac{\partial g}{\partial w_{n}}
\end{array}\right]
$$

## Optimization Procedure: Gradient Ascent

$$
\begin{aligned}
& \text { init } u \text { f } \\
& \text { for iter }=1,2 \text {, ... } \\
& \qquad w \leftarrow w+\alpha * \nabla g(w)
\end{aligned}
$$

- $\alpha$ : learning rate --- tweaking parameter that needs to be chosen carefully


## Batch Gradient Ascent on the Log Likelihood Objective

$$
\max _{w} l l(w)=\max _{w} \underbrace{\sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)}_{g(w)}
$$

$$
\begin{aligned}
& \text { init } u \\
& \text { for iter }=1,2, \ldots \\
& w \leftarrow w+\alpha * \sum_{i} \nabla \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
\end{aligned}
$$

## Stochastic Gradient Ascent on the Log Likelihood Objective

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

Observation: once gradient on one training example has been computed, might as well incorporate before computing next one

$$
\begin{aligned}
& \text { init } w \\
& \text { for iter }=1,2, \ldots \\
& \quad \text { pick random j } \\
& \quad w \leftarrow w+\alpha * \nabla \log P\left(y^{(j)} \mid x^{(j)} ; w\right)
\end{aligned}
$$

## Mini-Batch Gradient Ascent on the Log Likelihood Objective

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

Observation: gradient over small set of training examples (=mini-batch) can be computed in parallel, might as well do that instead of a single one

$$
\begin{aligned}
& \text { init } u \\
& \text { for iter }=1,2, \ldots \\
& \text { pick random subset of training examples J } \\
& \qquad w \leftarrow w+\alpha * \sum_{j \in J} \nabla \log P\left(y^{(j)} \mid x^{(j)} ; w\right)
\end{aligned}
$$

## What will gradient ascent do in multi-class logistic regression?

$$
\begin{aligned}
& w \leftarrow w+\alpha * \sum_{i} \nabla \log P\left(y^{(i)} \mid x^{(i)} ; w\right) \\
& P\left(y^{(i)} \mid x^{(i)} ; w\right)=\frac{e^{w_{y}(i) \cdot f\left(x^{(i)}\right)}}{\sum_{y} e^{w_{y} \cdot f\left(x^{(i)}\right)}} \\
& \begin{array}{l}
\nabla w_{y^{(i)}} f\left(x^{(i)}\right)-\nabla \log \sum_{y} e^{w_{y} f\left(x^{(i)}\right)} \\
\text { adds } \mathrm{f} \text { to the correct }
\end{array} \\
& \text { adds } \mathrm{f} \text { to the correct } \\
& \text { class weights } \\
& \frac{1}{\sum_{y} e^{w_{y} f\left(x^{(i)}\right)}} \sum_{y}\left(e^{w_{y} f\left(x^{(i)}\right)}\left[0^{T} f\left(x^{(i)}\right)^{T} 0^{T}\right]^{T}\right) \\
& \text { for } y^{\prime} \text { weights: } \frac{1}{\sum_{y} e^{w_{y} f\left(x^{(i)}\right)}} e^{w_{y^{\prime}} f\left(x^{(i)}\right)} f\left(x^{(i)}\right) \\
& P\left(y^{\prime} \mid x^{(i)} ; w\right) f\left(x^{(i)}\right) \quad \begin{array}{c}
\text { subtracts } \mathrm{f} \text { from } \mathrm{y}^{\prime} \text { weights in proportion to } \\
\text { the probability current weights give to } \mathrm{y}^{\prime}
\end{array}
\end{aligned}
$$

## Neural Networks



## Multi-class Logistic Regression

## = special case of neural network



## Deep Neural Network = Also learn the features!



## Deep Neural Network = Also learn the features!



$$
z_{i}^{(k)}=g\left(\sum_{j} W_{i, j}^{(k-1, k)} z_{j}^{(k-1)}\right)
$$

$\mathrm{g}=$ nonlinear activation function

## Deep Neural Network = Also learn the features!



$$
z_{i}^{(k)}=g\left(\sum_{j} W_{i, j}^{(k-1, k)} z_{j}^{(k-1)}\right)
$$

$\mathrm{g}=$ nonlinear activation function

## Common Activation Functions

Sigmoid Function


$$
g(z)=\frac{1}{1+e^{-z}}
$$

$$
g^{\prime}(z)=g(z)(1-g(z))
$$

Hyperbolic Tangent

$g(z)=\frac{e^{z}-e^{-z}}{e^{z}+e^{-z}}$
$g^{\prime}(z)=1-g(z)^{2}$

Rectified Linear Unit (ReLU)


$$
g(z)=\max (0, z)
$$

$g^{\prime}(z)=\left\{\begin{array}{lc}1, & z>0 \\ 0, & \text { otherwise }\end{array}\right.$

## Deep Neural Network: Also Learn the Features!

Training the deep neural network is just like logistic regression:

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

just $w$ tends to be a much, much larger vector
-> just run gradient ascent

+ stop when log likelihood of hold-out data starts to decrease


## Neural Networks Properties

Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.

## Practical considerations

Can be seen as learning the features
Large number of neurons
Danger for overfitting (hence early stopping!)

## Universal Function Approximation Theorem*

Hornik theorem 1: Whenever the activation function is bounded and nonconstant, then, for any finite measure $\mu$, standard multilayer feedforward networks can approximate any function in $L^{p}(\mu)$ (the space of all functions on $R^{k}$ such that $\int_{R^{k}}|f(x)|^{p} d \mu(x)<\infty$ ) arbitrarily well, provided that sufficiently many hidden units are available.

Hornik theorem 2: Whenever the activation function is continuous, bounded and nonconstant, then, for arbitrary compact subsets $X \subseteq R^{k}$, standard multilayer feedforward networks can approximate any continuous function on $X$ arbitrarily well with respect to uniform distance, provided that sufficiently many hidden units are available.

> In words: Given any continuous function $f(x)$, if a 2-layer neural network has enough hidden units, then there is a choice of weights that allow it to closely approximate $f(x)$.

## Universal Function Approximation Theorem*



Cybenko (1989) "Approximations by superpositions of sigmoidal functions" Hornik (1991) "Approximation Capabilities of Multilayer Feedforward Networks" Leshno and Schocken (1991) "Multilayer Feedforward Networks with Non-Polynomial Activation
Functions Can Approximate Any Function"

## How about computing all the derivatives?

Derivatives tables:

$$
\begin{array}{ll}
\frac{d}{d x}(a)=0 & \frac{d}{d x}[\ln u]=\frac{d}{d x}\left[\log _{e} u\right]=\frac{1}{u} \frac{d u}{d x} \\
\frac{d}{d x}(x)=1 & \frac{d}{d x}\left[\log _{a} u\right]=\log _{a} e \frac{1}{u} \frac{d u}{d x} \\
\frac{d}{d x}(a u)=a \frac{d u}{d x} & \frac{d}{d x} e^{u}=e^{u} \frac{d u}{d x} \\
\frac{d}{d x}(u+v-w)=\frac{d u}{d x}+\frac{d v}{d x}-\frac{d w}{d x} & \frac{d}{d x} a^{u}=a^{u} \ln a \frac{d u}{d x} \\
\frac{d}{d x}(u v)=u \frac{d v}{d x}+v \frac{d u}{d x} & \frac{d}{d x}\left(u^{v}\right)=v u^{v-1} \frac{d u}{d x}+\ln u u^{v} \frac{d v}{d x} \\
\frac{d}{d x}\left(\frac{u}{v}\right)=\frac{1}{v} \frac{d u}{d x}-\frac{u}{v^{2}} \frac{d v}{d x} & \frac{d}{d x} \sin u=\cos u \frac{d u}{d x} \\
\frac{d}{d x}\left(u^{n}\right)=n u^{n-1} \frac{d u}{d x} & \frac{d}{d x} \cos u=-\sin u \frac{d u}{d x} \\
\frac{d}{d x}(\sqrt{u})=\frac{1}{2 \sqrt{u} u} \frac{d u}{d x} & \frac{d}{d x} \tan u=\sec ^{2} u \frac{d u}{d x} \\
\frac{d}{d x}\left(\frac{1}{u}\right)=-\frac{1}{u^{2}} \frac{d u}{d x} & \frac{d}{d x} \cot u=-\csc 2 u \frac{d u}{d x} \\
\frac{d}{d x}\left(\frac{1}{u^{n}}\right)=-\frac{n}{u^{n+1}} \frac{d u}{d x} & \frac{d}{d x} \sec u=\sec ^{2} u \tan u \frac{d u}{d x} \\
\frac{d}{d x}[f(u)]=\frac{d}{d u}[f(u)] \frac{d u}{d x} & \frac{d}{d x} \csc u=-\csc u \cot u \frac{d u}{d x}
\end{array}
$$

## How about computing all the derivatives?

- But neural net $f$ is never one of those?
- No problem: CHAIN RULE:

If

$$
f(x)=g(h(x))
$$

Then

$$
f^{\prime}(x)=g^{\prime}(h(x)) h^{\prime}(x)
$$

Derivatives can be computed by following well-defined procedures

## Automatic Differentiation

## Automatic differentiation software

e.g. TensorFlow, PyTorch, Jax

Only need to program the function $g(x, y, w)$
Can automatically compute all derivatives w.r.t. all entries in w This is typically done by caching info during forward computation pass of $f$, and then doing a backward pass = "backpropagation"
Autodiff / Backpropagation can often be done at computational cost comparable to the forward pass

## Deep Neural Network = Also learn the features!



$$
z_{i}^{(k)}=g\left(\sum_{j} W_{i, j}^{(k-1, k)} z_{j}^{(k-1)}\right)
$$

$\mathrm{g}=$ nonlinear activation function

## Training a Network (setting weights)



Figure 21.3 (a) A neural network with two inputs, one hidden layer of two units, and one output unit. Not shown are the dummy inputs and their associated weights. (b) The network in (a) unpacked into its full computation graph.

## Back Propagation: $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$

- Suppose we have $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$ and want the gradient at $\boldsymbol{w}=[2,3]$
- Think of the function as a composition of many functions.
- Can use derivative chain rule to compute $\partial g / \partial w_{1}$ and $\frac{\partial g}{\partial w_{2}}$
- $\frac{\partial g}{\partial w_{1}}=$ $\qquad$

- More complex to compute for more complicated functions


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- $g=b+c$
- $\frac{\partial g}{\partial b}=1, \frac{\partial g}{\partial c}=1$


Computation Graph

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- $g=b+c$
- $\frac{\partial g}{\partial b}=1, \frac{\partial g}{\partial c}=1$
- $b=a \times w_{2}$
- $\frac{\partial g}{\partial a}=\frac{\partial g}{\partial b} \frac{\partial b}{\partial a}$



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- $b=a \times w_{2}$
- $\frac{\partial g}{\partial a}=\frac{\partial g}{\partial b} \frac{\partial b}{\partial a}=? ? ? ? ?$



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- $a=w_{1}^{3}$
- $\frac{\partial g}{\partial w_{1}}=$ ?????



## Back Propagation: $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$

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- $a=w_{1}^{3}$
- $\frac{\partial g}{\partial w_{1}}=\frac{\partial g}{\partial a} \frac{\partial a}{\partial w_{1}}=3 \cdot 3 w_{1}^{2}=36$

$$
\frac{\partial g}{\partial g}=1
$$

Interpretation: A tiny increase in $w_{1}$ will
result in an approximately 36 times
increase in $g$ due to this computation path.

## Back Propagation: $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$

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- $\frac{\partial g}{\partial w_{2}}=$ ? ?? $\quad$ Hint: $b=a \times 3$ may be useful.



## Back Propagation: $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$

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- $\frac{\partial g}{\partial a}=\frac{\partial g}{\partial b} \frac{\partial b}{\partial a}=1 \frac{\partial b}{\partial a}=1 \cdot 3=3$
- $\frac{\partial g}{\partial w_{2}}=\frac{\partial g}{\partial b} \frac{\partial b}{\partial w_{2}}=1 \frac{\partial b}{\partial w_{2}}=1 \cdot 8=8$
- $a=w_{1}^{3}$
- $\frac{\partial g}{\partial w_{1}}=\frac{\partial g}{\partial a} \frac{\partial a}{\partial w_{1}}=3 \cdot 3 w_{1}^{2}=36$



## Back Propagation: $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$

- Suppose we have $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$ and want the gradient at $\boldsymbol{w}=[2,3]$
- Think of the function as a composition of many functions, use chain rule.
- $g=b+c$
- $\frac{\partial g}{\partial b}=1, \frac{\partial g}{\partial c}=1$
- $b=a \times w_{2}$
- $\frac{\partial g}{\partial a}=\frac{\partial g}{\partial b} \frac{\partial b}{\partial a}=1 \frac{\partial b}{\partial a}=1 \cdot 3=3$
- $\frac{\partial g}{\partial w_{2}}=\frac{\partial g}{\partial b} \frac{\partial b}{\partial w_{2}}=1 \frac{\partial b}{\partial w_{2}}=1 \cdot 8=8$
- $a=w_{1}^{3}$

- $\frac{\partial g}{\partial w_{1}}=\frac{\partial g}{\partial a} \frac{\partial a}{\partial w_{1}}=3 \cdot 3 w_{1}^{2}=36$
- $c=3 w_{1}$
- $\frac{\partial g}{\partial w_{1}}=\frac{\partial g}{\partial c} \frac{\partial c}{\partial w_{1}}=1 \cdot 3=3$

Adding the changes to g contributed by change in $\mathrm{w}_{1}$ together

## Back Propagation: $g(\boldsymbol{w})=w_{1}^{3} w_{2}+3 w_{1}$

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- $c=3 w_{1}$
- $\frac{\partial g}{\partial w_{1}}=\frac{\partial g}{\partial c} \frac{\partial c}{\partial w_{1}}=1 \cdot 3=3$


$$
\nabla g=\left[\frac{\partial g}{\partial w_{1}}, \frac{\partial g}{\partial w_{2}}\right]=[39,8]
$$



## Summary of Key Ideas

Optimize probability of label given input $\quad \max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)$

## Continuous optimization

Gradient ascent:
Compute steepest uphill direction = gradient (= just vector of partial derivatives)
Take step in the gradient direction
Repeat (until held-out data accuracy starts to drop = "early stopping")

## Deep neural nets

Last layer $=$ still logistic regression
Now also many more layers before this last layer
= computing the features
the features are learned rather than hand-designed
Universal function approximation theorem
If neural net is large enough
Then neural net can represent any continuous mapping from input to output with arbitrary accuracy
But remember: need to avoid overfitting / memorizing the training data $\rightarrow$ early stopping!
Automatic differentiation gives the derivatives efficiently

## How well does it work?

Computer Vision


## Object Detection



## Manual Feature Design



## Features and Generalization



## Features and Generalization



Image


HoG

## Performance

## ImageNet Error Rate 2010-2014



## Performance

## ImageNet Error Rate 2010-2014



## Performance

## ImageNet Error Rate 2010-2014



## Performance

## ImageNet Error Rate 2010-2014



## Performance

## ImageNet Error Rate 2010-2014



## MS COCO Image Captioning Challenge


"man in black shirt is playing guitar."

"girl in pink dress is jumping in air."

"construction worker in orange safety vest is working on road.

"black and white dog jumps over bar."

"two young girls are playing with lego toy."

"young girl in pink shirt is swinging on swing."

"boy is doing backflip on wakeboard."

"man in blue wetsuit is surfing on wave."

Karpathy \& Fei-Fei, 2015; Donahue et al., 2015; Xu et al, 2015; many more

## Visual QA Challenge



## Image Segmentation



## Speech Recognition

## TIMIT Speech Recognition

- Traditional Deep Learning



## Machine Translation

Google Neural Machine Translation (in production)

Encoder


## CheXNet: Radiologist-Level Pneumonia Detection on Chest XRays with Deep Learning

Pranav Rajpurkar*, Jeremy Irvin*, Kaylie Zhu, Brandon Yang, Hershel Mehta, Tony Duan, Daisy Ding, Aarti Bagul, Curtis Langlotz, Katie Shpanskaya, Matthew P. Lungren, Andrew Y. Ng

We develop an algorithm that can detect pneumonia from chest X -rays at a level exceeding practicing radiologists.

Chest X-rays are currently the best available method for diagnosing pneumonia, playing a crucial role in clinical care and epidemiological studies. Pneumonia is responsible for more than 1 million hospitalizations and 50,000 deaths per year in the US alone.


## Google and DeepMind are using AI to predict the energy output of wind farms

To help make that energy more valuable to the power grid
By Nick Statt | @nickstatt | Feb 26, 2019, 2:42pm EST
f $\quad \underbrace{\text { share }}$


Google announced today that it has made energy produced by wind farms more viable using the artificial intelligence software of its London-based subsidiary DeepMind. By using DeepMind's machine learning algorithms to predict the wind output from the farms Google uses for its green energy initiatives, the company says it can now schedule set deliveries of energy output, which are more valuable to the grid than standard, non-time-based deliveries.

## Change in Programming Paradigm!

## Traditional Programming:

 program by writing lines of code

Poor performance on Al problems

Deep Learning ("Software 2.0"): program by providing data


Success!

