Announcement

- **Slides for Catherine Olsson's guest lecture**
	- Please reach out to catherio@anthropic.com
- **Another guest lecture by Miles Brundage** break (Dec 3)

CS 188: Artificial Intelligence

Neural Networks and Optimization

[These slides were created by Dan Klein, Pieter Abbeel, Anca Dragan for CS188 Intro to AI at UC Berkeley. All CS188 materials are available at http://ai.berkeley.edu.]

Image Classification

$$
h_i^{(l)} = \phi(\sum_j w_{ji}^{(l)} \cdot h_j^{(l-1)})
$$

$$
\phi = \text{activation function}
$$

- Neural network with L layers
- $h^{(l)}$: activations at layer I
- $w^{(l)}$: weights taking activations from layer l-1 to layer l

Recap: Common Activation Functions ϕ

Sigmoid Function

Rectified Linear Unit (ReLU)

 $g'(z) = g(z)(1 - g(z))$

 $g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$

Neural Network Shapes

Take d-dimensional input vector x and calculate first hidden unit vector h⁽¹⁾

Shape (1,n) vector

Shape (d,n) matrix

$$
h^{(1)} = \phi(x \times W^{(1)})
$$

Shape (1,d) vector

Calculate next hidden unit vector $h^{(l)}$ from previous $h^{(l-1)}$

Shape (1,n) vector Shape (n,n) matrix

$$
h^{(l)} = \phi(h^{(l-1)} \times W^{(l)})
$$

Shape (1,n) vector

Calculate final k-dimensional vector z (and pass to softmax to get $p(y|x)$)

Shape (1,k) vector

Shape (n,k) matrix

$$
z = \phi(h^{(L)} \times W^{(out)})
$$

Shape (1,n) vector

Example: Sizes of neural networks

We have a neural network with the matrices drawn.

- 1. How many layers are in the network?
- 2. How many input dimensions d?
- 3. How many hidden neurons n?
- 4. How many output dimensions k?

Example: Sizes of neural networks

We have a neural network with the matrices drawn.

- 1. How many layers are in the network? 1
- 2. How many input dimensions d? 3
- 3. How many hidden neurons n? 2
- 4. How many output dimensions k? 1

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.

Universal Function Approximation Theorem*

Hornik theorem 1: Whenever the activation function is bounded and nonconstant, then, for any finite measure μ , 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.

 \blacksquare 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).

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"

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"

- With non-linear activation ϕ for intermediate output: $y = \phi(w_1h_1 + w_2h_2)$ $= \phi(w_1\phi(w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + w_2\phi(w_{12}x_1 + w_{22}x_2 + w_{32}x_3))$
- **Without** intermediate activations ϕ :
- $y = \phi(w_1(w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + w_2(w_{12}x_1 + w_{22}x_2 + w_{32}x_3))$ $= \phi((w_1w_{11} + w_2w_{12})x_1 + (w_1w_{21} + w_2w_{22})x_2 + (w_1w_{31} + w_2w_{32})x_3)$ $\phi = \phi(ax_1 + bx_2 + cx_3)$ \leftrightarrow same as not including a hidden layer!

Deep Neural Network Training

■ Training the deep neural network is just like logistic regression -Maximize log of likelihood of the data:

$$
\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$

- **For each training example (i), maximize probability of label y(i) given input x(i)**
- Parameter w tends to be a much, much larger vector
- How do we maximize w?
	- Numerical optimization (i.e. hill climbing)

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 logistic regression or neural networks?
	- Optimization over a continuous space
		- Infinitely many neighbors!
		- How to do this efficiently?

Review: Derivatives and Gradients

■ What is the derivative of the function $g(x) = x^2 + 3$?

$$
\frac{dg}{dx} = 2x
$$

• What is the derivative of $g(x)$ at $x=5$?

$$
\frac{dg}{dx}|_{x=5} = 10
$$

Review: Derivatives and Gradients

- What is the gradient of the function $g(x,y) = x^2y$?
	- Recall: Gradient is a vector of partial derivatives with respect to each variable

$$
\nabla g = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2xy \\ x^2 \end{bmatrix}
$$

• What is the derivative of $g(x, y)$ at $x=0.5$, $y=0.5$?

$$
\nabla g|_{x=0.5, y=0.5} = \begin{bmatrix} 2(0.5)(0.5) \\ (0.5^2) \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.25 \end{bmatrix}
$$

1-D Optimization

• Could evaluate $g(w_0 + h)$ and $g(w_0 - h)$

- Then step in best direction
- Or, evaluate derivative:

$$
\frac{\partial g(w_0)}{\partial w} = \lim_{h \to 0} \frac{g(w_0 + h) - g(w_0 - h)}{2h}
$$

■ 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:** $g(w_1, w_2)$
	- Updates:

$$
w_1 \leftarrow w_1 + \alpha * \frac{\partial g}{\partial w_1}(w_1, w_2)
$$

$$
w_2 \leftarrow w_2 + \alpha * \frac{\partial g}{\partial w_2}(w_1, w_2)
$$

■ Updates in vector notation:

$$
w \leftarrow w + \alpha * \nabla_w g(w)
$$

$$
\text{with: } \nabla_w g(w) = \begin{bmatrix} \frac{\partial g}{\partial w_1}(w) \\ \frac{\partial g}{\partial w_2}(w) \end{bmatrix}
$$

= gradient

Gradient Ascent

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

Figure source: Mathworks

Gradient Ascent

§ Idea:

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

Figure source: Mathworks

Gradient in n dimensions

$$
\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \\ \dots \\ \frac{\partial g}{\partial w_n} \end{bmatrix}
$$

Optimization Procedure: Gradient Ascent

$$
\begin{array}{ll}\n\text{Init } w \\
\text{for iter} = 1, 2, \dots \\
\text{w} \leftarrow w + \alpha \cdot \nabla g(w)\n\end{array}
$$

- \bullet α : learning rate --- tweaking parameter that needs to be chosen carefully
- **EXED:** How? Try multiple choices
	- Crude rule of thumb: update changes w about $0.1 1$ %

Learning Rate

Choice of learning rate α is a hyperparameter Example: α =0.001 (too small)

Learning Rate

Choice of step size α is a hyperparameter Example: α =0.004 (too large)

Source: https://distill.pub/2017/momentum/

Gradient Ascent with Momentum*

■ Often use *momentum* to improve gradient ascent convergence

Init w for iter = $1, 2, ...$ $w \leftarrow w + \alpha \cdot \nabla g(w)$

Gradient Ascent: Gradient Ascent with momentum:

- One interpretation: *w* moves like a particle with mass
- Another: *exponential moving average* on gradient

Gradient Ascent with Momentum*

Example: α =0.001 and β =0.0

Source: https://distill.pub/2017/momentum/

Gradient Ascent with Momentum*

Example: α =0.001 and β =0.9

Source: https://distill.pub/2017/momentum/

Batch Gradient Ascent on the Log Likelihood Objective

$$
\max_{w} \quad ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$
\n
$$
g(w)
$$

\n- $$
\blacksquare
$$
 int w
\n- \blacksquare for iter = 1, 2, ...
\n- $w \leftarrow w + \alpha * \sum_{i} \nabla \log P(y^{(i)} | x^{(i)}; w)$
\n

Sum rule for derivatives: derivative of $[a(w) + b(w)] =$ derivative of $a(w) +$ derivative of $b(w)$

Stochastic Gradient Ascent on the Log Likelihood Objective

$$
\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$

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

\n- init
$$
w
$$
\n- for $iter = 1, 2, \ldots$
\n- pick random j
\n- $w \leftarrow w + \alpha * \nabla \log P(y^{(j)} | x^{(j)}; w)$
\n

Mini-Batch Gradient Ascent on the Log Likelihood Objective

$$
\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$

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

\n- init
$$
w
$$
\n- for $iter = 1, 2, \ldots$
\n- pick random subset of training examples J
\n- $w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)} | x^{(j)}; w)$
\n

How about computing all the derivatives?

Derivatives tables:

$$
\frac{d}{dx}(a) = 0 \qquad \frac{d}{dx}[\ln u] = \frac{d}{dx}[\log_e u] = \frac{1}{u}\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(au) = a\frac{du}{dx} \qquad \frac{d}{dx}e^u = e^u\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(u+v-w) = \frac{du}{dx} + \frac{dv}{dx} - \frac{dw}{dx} \qquad \frac{d}{dx}a^u = a^u \ln a \frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx} \qquad \frac{d}{dx}(u^v) = vu^{v-1}\frac{du}{dx} + \ln u \quad u^v\frac{dv}{dx}
$$
\n
$$
\frac{d}{dx}(\frac{u}{v}) = \frac{1}{v}\frac{du}{dx} - \frac{u}{v^2}\frac{dv}{dx} \qquad \frac{d}{dx}\sin u = \cos u\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(u^n) = nu^{n-1}\frac{du}{dx} \qquad \frac{d}{dx}\cos u = -\sin u\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(\sqrt{u}) = \frac{1}{2\sqrt{u}}\frac{du}{dx} \qquad \frac{d}{dx}\tan u = \sec^2 u\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(\frac{1}{u}) = -\frac{1}{u^2}\frac{du}{dx} \qquad \frac{d}{dx}\cot u = -\csc^2 u\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}(\frac{1}{u^n}) = -\frac{n}{u^{n+1}}\frac{du}{dx} \qquad \frac{d}{dx}\cot u = -\csc^2 u\frac{du}{dx}
$$
\n
$$
\frac{d}{dx}[f(u)] = \frac{d}{du}[f(u)]\frac{du}{dx} \qquad \frac{d}{dx}\csc u = -\csc u\cot u\frac{du}{dx}
$$

How about computing all the derivatives?

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

$$
\text{If} \quad f(x) = g(h(x))
$$

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

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
- Need to know this exists

How this is done? Details outside of scope of CS188, but we'll show a basic example

Backpropagation*

- Gradient of $g(w_1, w_2, w_3) = w_1^4 w_2 + 5 w_3$ at $w_1 = 2$, $w_2 = 3$, $w_3 = 2$
- Think of *g* as a composition of many functions
	- Then, we can use the chain rule to compute the gradient
- $g = b + c$
	- $\frac{\partial g}{\partial b} = 1, \frac{\partial g}{\partial c} = 1$
- $b = a \times w_2$

$$
\frac{\partial g}{\partial a} = \frac{\partial g}{\partial b} \frac{\partial b}{\partial a} = 1 \cdot w_2 = 3 \qquad \frac{\partial g}{\partial w_2} = \frac{\partial g}{\partial b} \frac{\partial b}{\partial w_2} = 1 \cdot a = 16
$$

$$
a = w_1^4
$$

$$
\frac{\partial g}{\partial w_1} = \frac{\partial g}{\partial a} \frac{\partial a}{\partial w_1} = 3 \cdot 4w_1^3 = 96
$$

$$
c = 5w_1
$$

$$
\frac{\partial g}{\partial w_3} = \frac{\partial g}{\partial c} \frac{\partial c}{\partial w_3} = 1 \cdot 5 = 5
$$

Preventing Overfitting in Optimization

Weight regularization

Weight Regularization

What can go wrong when we maximize log-likelihood? Example: logistic regression with only one datapoint: $f(x)=1$, $y=+1$

w can grow very large and lead to overfitting and learning instability

Weight Regularization

What can go wrong when we maximize log-likelihood?

$$
\max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$

w can grow very large

Solution: add an objective term to penalize weight magnitude max_{w} \boldsymbol{i} $\log P(y^{(i)} | x^{(i)}; w) - \frac{\lambda}{2}$ $\frac{1}{2}$ \boldsymbol{j} w_j^2

 λ is a hyperparameter (typically 0.1 to 0.0001 or smaller)

Consistency vs. Simplicity

■ Example: curve fitting (regression, function approximation)

- Consistency vs. simplicity
- Ockham's razor

Consistency vs. Simplicity

- Usually algorithms prefer consistency by default (why?)
- Several ways to operationalize "simplicity"
	- Reduce the hypothesis/model space
		- Assume more: e.g. independence assumptions, as in naïve Bayes
		- Fewer features or neurons
		- Other limits on model structure
	- Regularization
		- Laplace Smoothing: cautious use of small counts
		- Small weight vectors in neural networks (stay close to zero-mean prior)
		- Hypothesis space stays big, but harder to get to the outskirts

Fun Neural Net Dem

Demo-site: http://playground.tensorflow.org/

Neural Networks: Summary of Key Ideas

Optimize probability of label given input

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 ? early stopping!

Automatic differentiation gives the derivatives efficiently (how? = outside of scope of 188)

 $\max_{w} \; l l(w) = \max_{w} \; \sum_{z} \log P(y^{(i)} | x^{(i)}; w)$

Next: Applications and Putting it all together!

