CS224d
Deep NLP

Lecture 4:
Word Window Classification and Neural Networks

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Overview Today:

- General classification background
- Updating word vectors for classification
- Window classification & cross entropy error derivation tips
- A single layer neural network!
- (Max-Margin loss and **backprop**)

Classification setup and notation

- Generally we have a training dataset consisting of samples

$$\{x_i, y_i\}^N_{i=1}$$

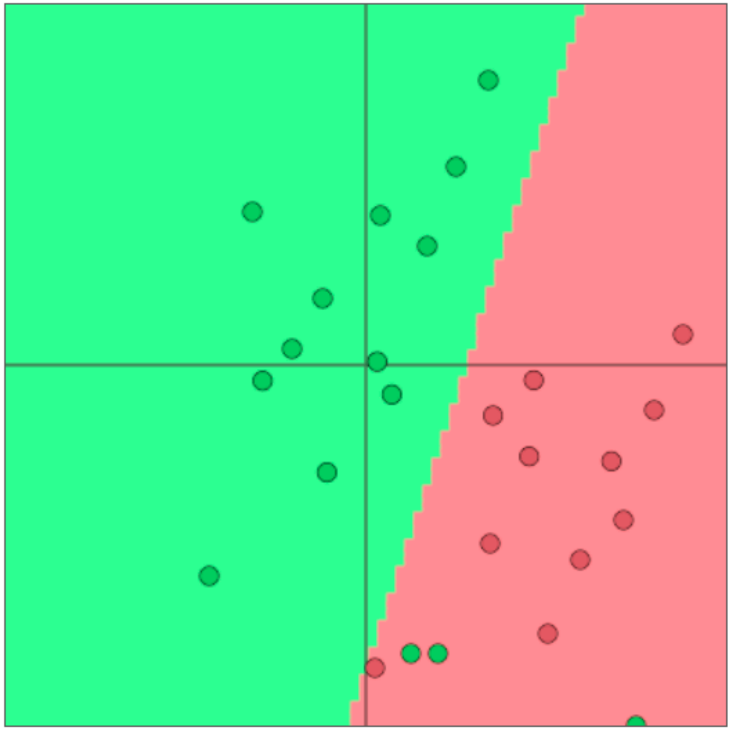
- x_i - inputs, e.g. words (indices or vectors!), context windows, sentences, documents, etc.

- y_i - labels we try to predict,
  - e.g. other words
  - class: sentiment, named entities, buy/sell decision,
  - later: multi-word sequences

Classification intuition

- Training data: $\{x_i, y_i\}^N_{i=1}$
- Simple illustration case:
  - Fixed 2d word vectors to classify
  - Using logistic regression
  - → linear decision boundary →
- General ML: assume x is fixed and only train logistic regression weights W and only modify the decision boundary

$$p(y|x) = \frac{\exp(W_y.x)}{\sum_{c=1}^{C} \exp(W_c.x)}$$

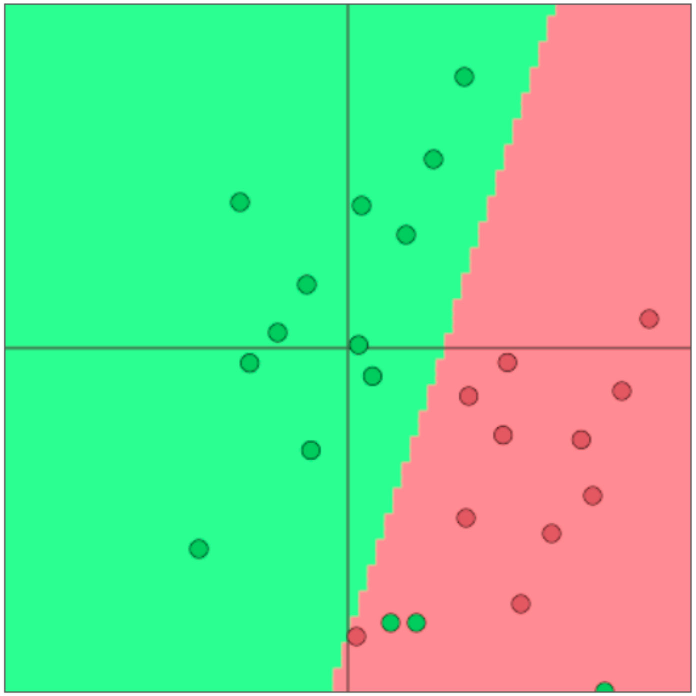


Visualizations with ConvNetJS by Karpathy!
http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html

Classification notation

- Cross entropy loss function over dataset $\{x_i,y_i\}^N_{i=1}$

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} -\log\left(\frac{e^{f_{y_i}}}{\sum_{c=1}^{C} e^{f_c}}\right)$$



- Where for each data pair (x_i,y_i):

$$f_y = f_y(x) = W_{y\cdot}x = \sum_{j=1}^{d} W_{yj}x_j$$

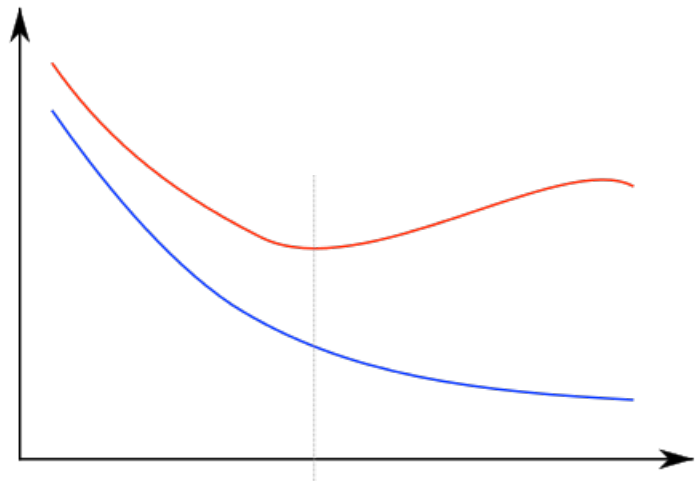
- We can write *f* in matrix notation and index elements of it based on class: $f = Wx$

Classification: Regularization!

- Really full loss function over any dataset includes **regularization** over all parameters μ:

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} -\log\left(\frac{e^{f_{y_i}}}{\sum_{c=1}^{C} e^{f_c}}\right) + \lambda \sum_k \theta_k^2$$

- Regularization will prevent overfitting when we have a lot of features (or later a very powerful/deep model)
  - x-axis: more powerful model or more training iterations
  - Blue: training error, red: test error

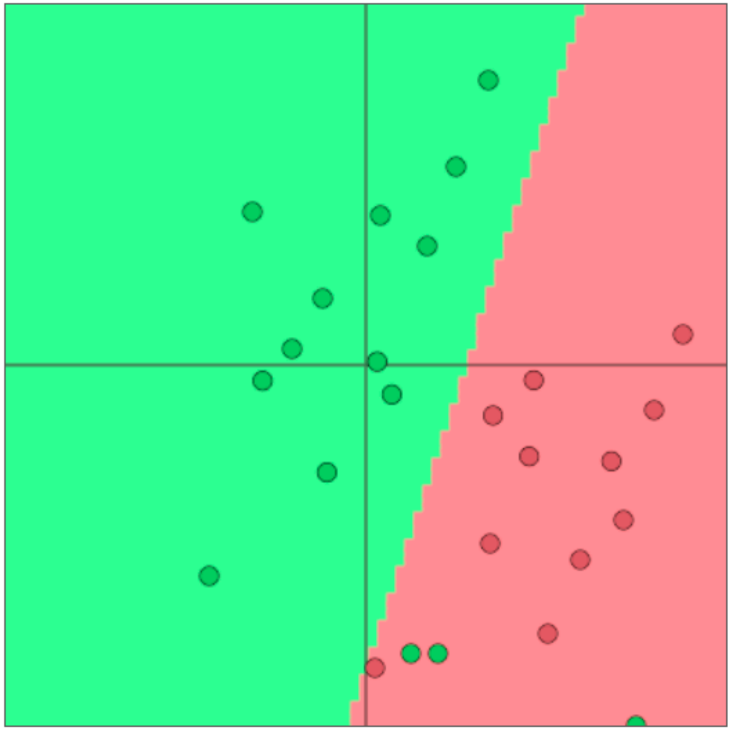


Details: General ML optimization

- For general machine learning μ usually only consists of columns of W:

$$\theta = \begin{bmatrix} W_{\cdot 1} \\ \vdots \\ W_{\cdot d} \end{bmatrix} = W(:) \in \mathbb{R}^{Cd}$$

C --> Number of classes
d --> X dimensionality



Visualizations with ConvNetJS by Karpathy

- So we only update the decision boundary

$$\nabla_\theta J(\theta) = \begin{bmatrix} \nabla_{W_{\cdot 1}} \\ \vdots \\ \nabla_{W_{\cdot d}} \end{bmatrix} \in \mathbb{R}^{Cd}$$

Classification difference with word vectors

- Common in deep learning:
  - Learn both W and word vectors x

$$\nabla_\theta J(\theta) = \begin{bmatrix} \nabla_{W_{\cdot 1}} \\ \vdots \\ \nabla_{W_{\cdot d}} \\ \nabla_{x_{aardvark}} \\ \vdots \\ \nabla_{x_{zebra}} \end{bmatrix} \in \mathbb{R}^{Cd+\boxed{Vd}}$$

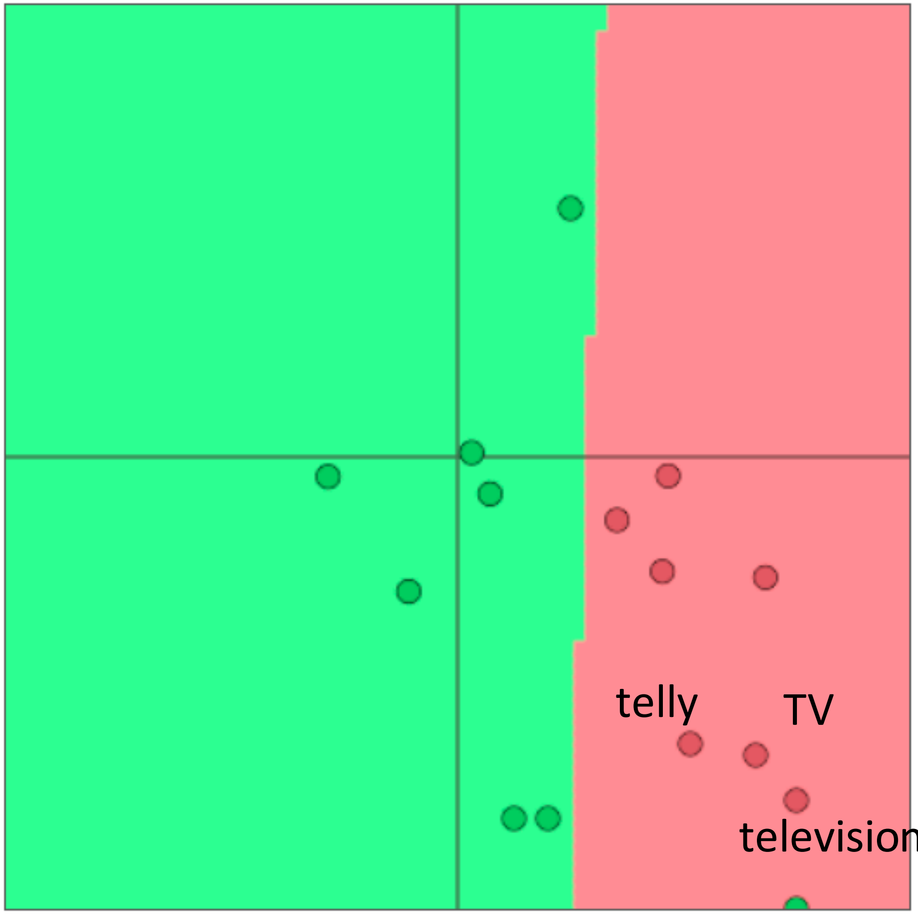
Very large!

Overfitting Danger!

Losing generalization by re-training word vectors

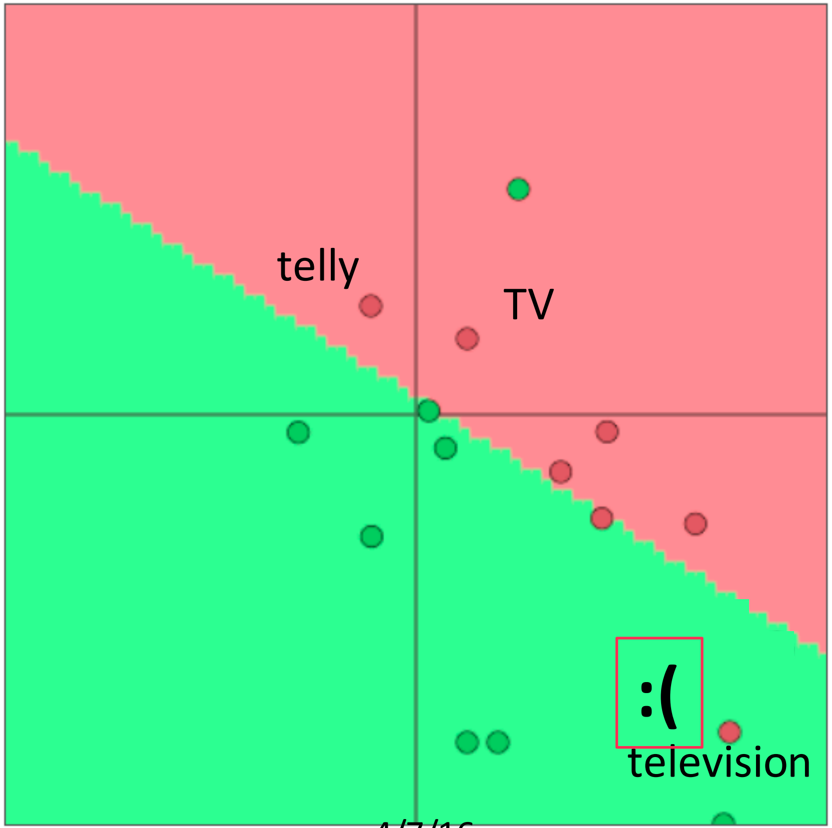
- Setting: Training logistic regression for movie review sentiment and in the training data we have the words
  - "TV" and "telly"
- In the testing data we have
  - "television"
- Originally they were all similar (from pre-training word vectors)

- What happens when we train the word vectors?



Losing generalization by re-training word vectors

- What happens when we train the word vectors?
  - Those that are in the training data move around
  - Words from pre-training that do NOT appear in training stay



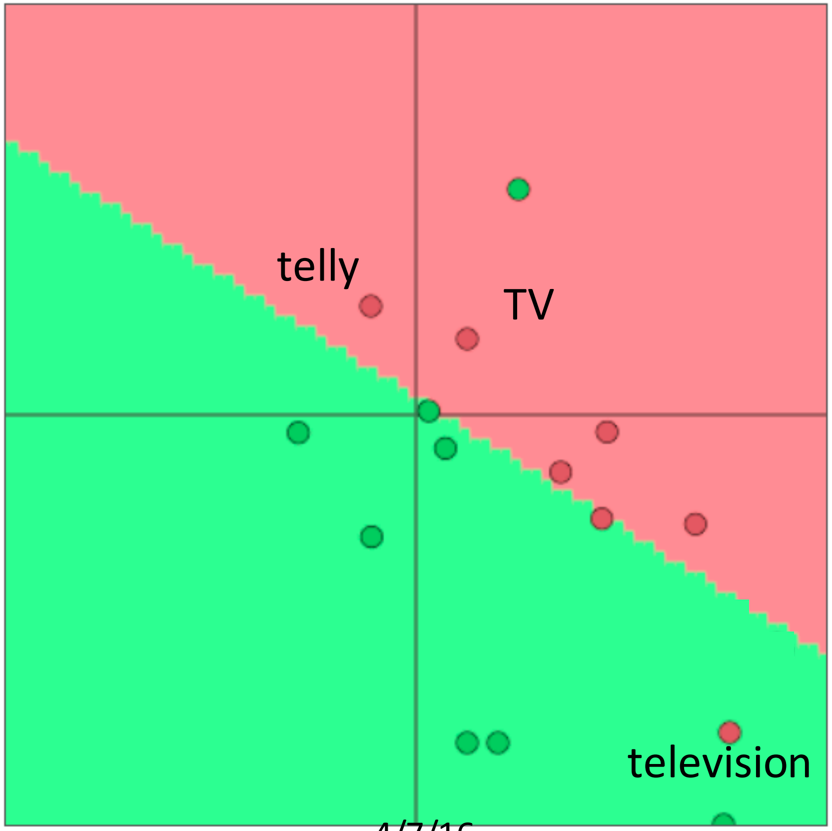
- Example:
- In training data: “TV” and “telly”
- In testing data only: “television”

Losing generalization by re-training word vectors

- Take home message:

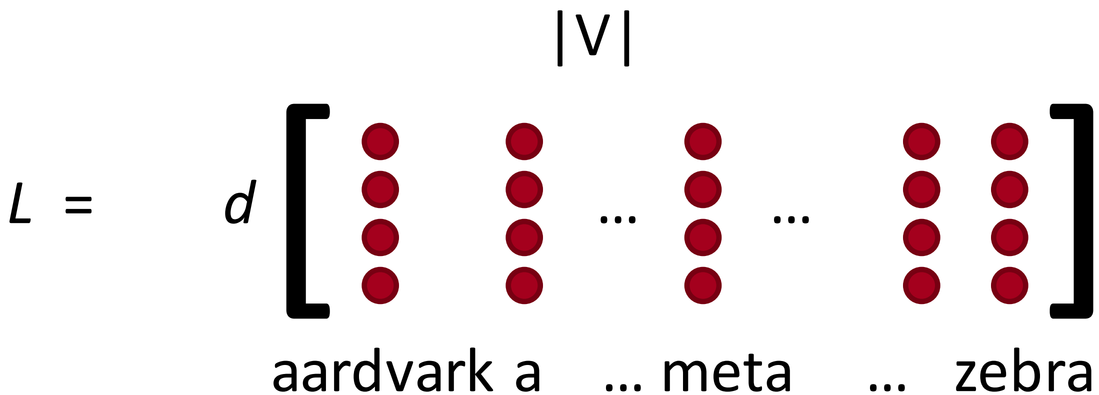
If you only have a small training data set, don't train the word vectors.

If you have have a very large dataset, it may work better to train word vectors to the task.



Side note on word vectors notation

- The word vector matrix L is also called lookup table
- Word vectors = word embeddings = word representations (mostly)
- Mostly from methods like word2vec or Glove



- These are the word features x_{word} from now on

- Conceptually you get a word's vector by left multiplying a one-hot vector *e* by *L*: *x = Le 2 d£ V ¢ V £ 1*

Window classification

- Classifying single words is rarely done.

- Interesting problems like ambiguity arise in context!

- Example: auto-antonyms:
  - "To sanction" can mean "to permit" or "to punish.”
  - "To seed" can mean "to place seeds" or "to remove seeds."

- Example: ambiguous named entities:
  - Paris → Paris, France vs Paris Hilton
  - Hathaway → Berkshire Hathaway vs Anne Hathaway

Window classification

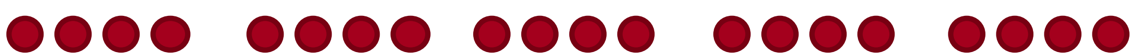
- Idea: classify a word in its context window of neighboring words.
- For example named entity recognition into 4 classes:
  - Person, location, organization, none
- Many possibilities exist for classifying one word in context, e.g. averaging all the words in a window but that looses position information

Window classification

- Train softmax classifier by assigning a label to a center word and concatenating all word vectors surrounding it

- Example: Classify Paris in the context of this sentence with window length 2:

… museums in Paris are amazing … .



$X_{window} = [\ x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing}\ ]^T$

- Resulting vector $x_{window} = \boxed{x \in R^{5d}}$, a column vector!

Simplest window classifier: Softmax

- With $x = x_{window}$ we can use the same softmax classifier as before

predicted model output probability

$$\boxed{\hat{y}_y} = p(y|x) = \frac{\exp(\boxed{W_{y\cdot}x})}{\sum_{c=1}^{C}\exp(W_{c\cdot}x)}$$

- With cross entropy error as before:

same

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} -\log\left(\frac{e^{\boxed{f_{y_i}}}}{\sum_{c=1}^{C} e^{f_c}}\right)$$

- But how do you update the word vectors?

Updating concatenated word vectors

- Short answer: Just take derivatives as before

- Long answer: Let's go over the steps together (you'll have to fill in the details in PSet 1!)
- Define:
    - $\hat{y}$: softmax probability output vector (see previous slide)
    - t: target probability distribution (all 0's except at ground truth index of class y, where it's 1)
    - $f = f(x) = Wx \in \mathbb{R}^C$ and f_c = c'th element of the f vector

- Hard, the first time, hence some tips now :)

Updating concatenated word vectors

- Tip 1: Carefully define your variables and keep track of their dimensionality!

$$f = f(x) = Wx \in \mathbb{R}^C$$

$$\hat{y} \quad t \qquad W \in \mathbb{R}^{C \times 5d}$$

- Tip 2: **Know thy chain rule** and don't forget which variables depend on what:

$$\frac{\partial}{\partial x} - \log softmax(f_y(x)) = \sum_{c=1}^{C} - \frac{\partial \log softmax(f_y(x))}{\partial f_c} \cdot \frac{\partial f_c(x)}{\partial x}$$

- Tip 3: For the softmax part of the derivative: First take the derivative wrt f_c when c=y (the correct class), then take derivative wrt f_c when c≠ y (all the incorrect classes)

Updating concatenated word vectors

- Tip 4: When you take derivative wrt one element of f, try to see if you can create a gradient in the end that includes all partial derivatives:

$$\hat{y} \qquad t$$

$$f = f(x) = Wx \in \mathbb{R}^C$$

$$\frac{\partial}{\partial f} - \log softmax(f_y) = \begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_y - 1 \\ \vdots \\ \hat{y}_C \end{bmatrix}$$

- Tip 5: To later not go insane & implementation! → results in terms of vector operations and define single index-able vectors:

$$\frac{\partial}{\partial f} - \log softmax(f_y) = [\hat{y} - t] = \delta$$

Updating concatenated word vectors

- Tip 6: When you start with the chain rule, first use explicit sums and look at partial derivatives of e.g. x_i or W_{ij}

$$\hat{y} \qquad t$$

$$f = f(x) = Wx \in \mathbb{R}^C$$

$$\sum_{c=1}^{C} -\frac{\partial \log softmax(f_y(x))}{\partial f_c} \cdot \frac{\partial f_c(x)}{\partial x} = \sum_{c=1}^{C} \delta_c W_{c\cdot}^T$$

- Tip 7: To clean it up for even more complex functions later: Know dimensionality of variables &simplify into matrix notation

$$\frac{\partial}{\partial x} - \log p(y|x) = \sum_{c=1}^{C} \delta_c W_{c\cdot}^T = W^T \delta$$

- Tip 8: Write this out in full sums if it's not clear!

Updating concatenated word vectors

- What is the dimensionality of the window vector gradient?

$$\frac{\partial}{\partial x} - \log p(y|x) = \sum_{c=1}^{C} \delta_c W_{c\cdot} = W^T \delta$$

- x is the entire window, 5 d-dimensional word vectors, so the derivative wrt to x has to have the same dimensionality:

$$\nabla_x J = W^T \delta \in \mathbb{R}^{5d}$$

Updating concatenated word vectors

- The gradient that arrives at and updates the word vectors can simply be split up for each word vector:
- Let $\nabla_x J = W^T \delta = \delta_{x_{window}}$
- With x_{window} = [$x_{museums}$ x_{in} x_{Paris} x_{are} $x_{amazing}$]
- We have

$$\delta_{window} = \begin{bmatrix} \nabla_{x_{museums}} \\ \nabla_{x_{in}} \\ \nabla_{x_{Paris}} \\ \nabla_{x_{are}} \\ \nabla_{x_{amazing}} \end{bmatrix} \in \mathbb{R}^{5d}$$

Updating concatenated word vectors

- This will push word vectors into areas such they will be helpful in determining named entities.

- For example, the model can learn that seeing x_{in} as the word just before the center word is indicative for the center word to be a location

What's missing for training the window model?

- The gradient of J wrt the softmax weights W!

- Similar steps, write down partial wrt W_{ij} first!
- Then we have full

$$\nabla_\theta J(\theta) = \begin{bmatrix} \nabla_{W_{\cdot 1}} \\ \vdots \\ \nabla_{W_{\cdot d}} \\ \nabla_{x_{aardvark}} \\ \vdots \\ \nabla_{x_{zebra}} \end{bmatrix} \in \mathbb{R}^{Cd+Vd}$$

A note on matrix implementations

- There are two expensive operations in the softmax:
- The matrix multiplication $f = Wx$ and the exp
- A for loop is never as efficient when you implement it compared vs when you use a larger matrix multiplication!

- Example code →

A note on matrix implementations

- Looping over word vectors instead of concatenating them all into one large matrix and then multiplying the softmax weights with that matrix

```
from numpy import random
N = 500 # number of windows to classify
d = 300 # dimensionality of each window
C = 5 # number of classes
W = random.rand(C,d)
wordvectors_list = [random.rand(d,1) for i in range(N)]
wordvectors_one_matrix = random.rand(d,N)

%timeit [W.dot(wordvectors_list[i]) for i in range(N)]
%timeit W.dot(wordvectors_one_matrix)
```

- 1000 loops, best of 3: 639 µs per loop
  10000 loops, best of 3: 53.8 µs per loop

A note on matrix implementations

```
from numpy import random
N = 500 # number of windows to classify
d = 300 # dimensionality of each window
C = 5 # number of classes
W = random.rand(C,d)
wordvectors_list = [random.rand(d,1) for i in range(N)]
wordvectors_one_matrix = random.rand(d,N)

%timeit [W.dot(wordvectors_list[i]) for i in range(N)]
%timeit W.dot(wordvectors_one_matrix)
```

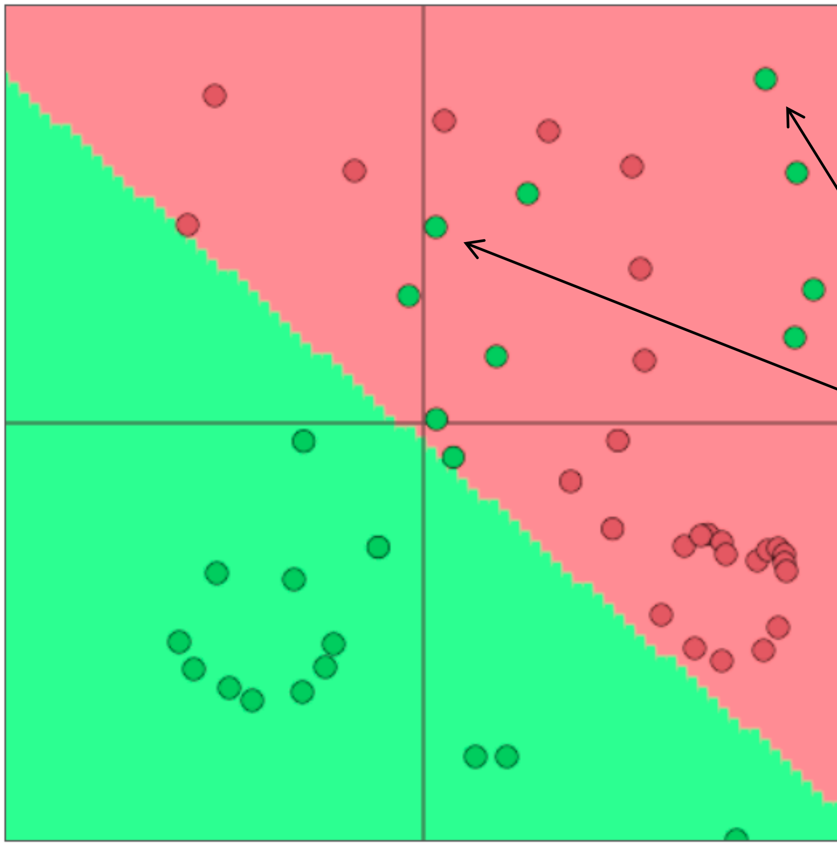
- Result of faster method is a C x N matrix:
  - Each column is an f(x) in our notation (unnormalized class scores)
- Matrices are awesome!
- You should speed test your code a lot too

Softmax (= logistic regression) is not very powerful

- Softmax only gives linear decision boundaries in the original space.
- With little data that can be a good regularizer
- With more data it is very limiting!

Softmax (= logistic regression) is not very powerful

- Softmax only linear decision boundaries

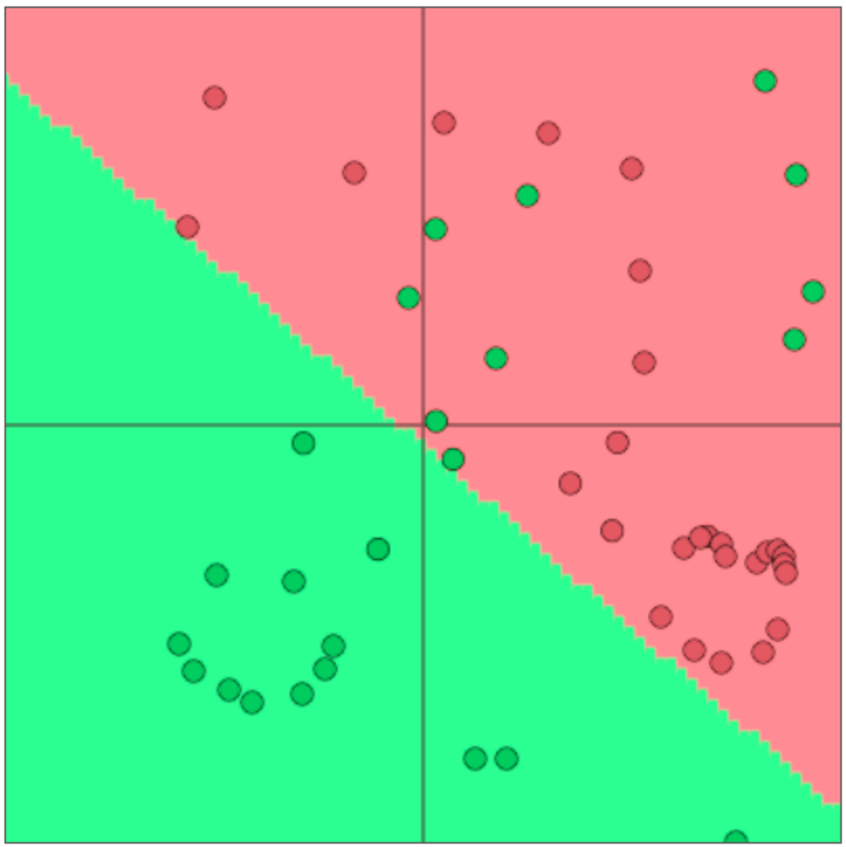


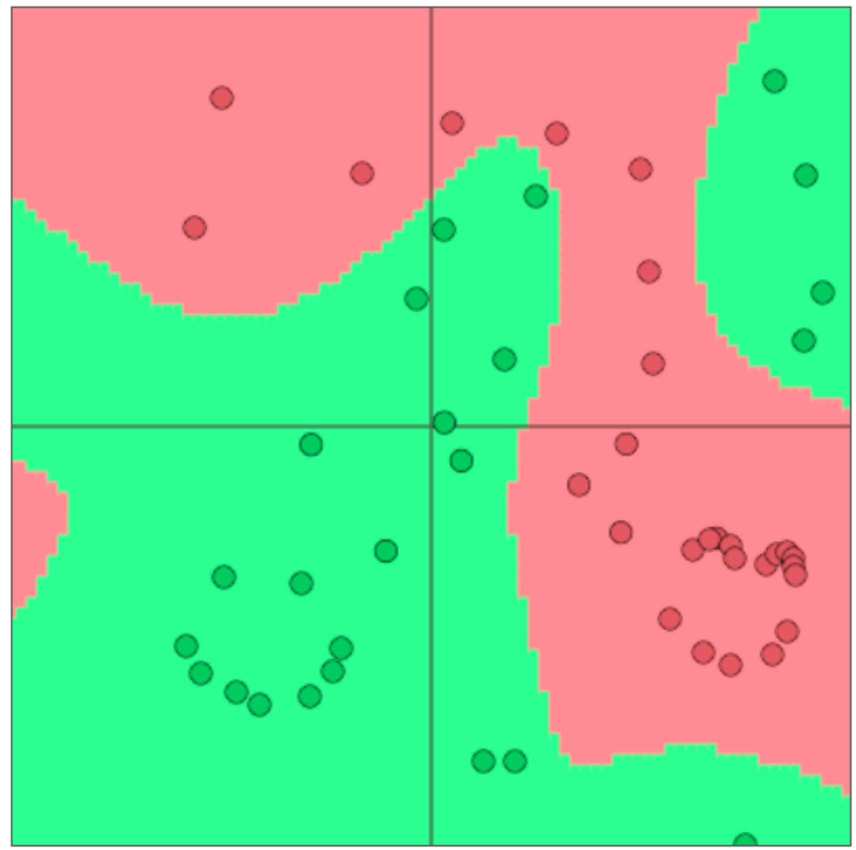
→ Lame when problem is complex

Wouldn't it be cool to get these correct?

Neural Nets for the Win!

- Neural networks can learn much more complex functions and nonlinear decision boundaries!





From logistic regression to neural nets

Demystifying neural networks

Neural networks come with their own terminological baggage

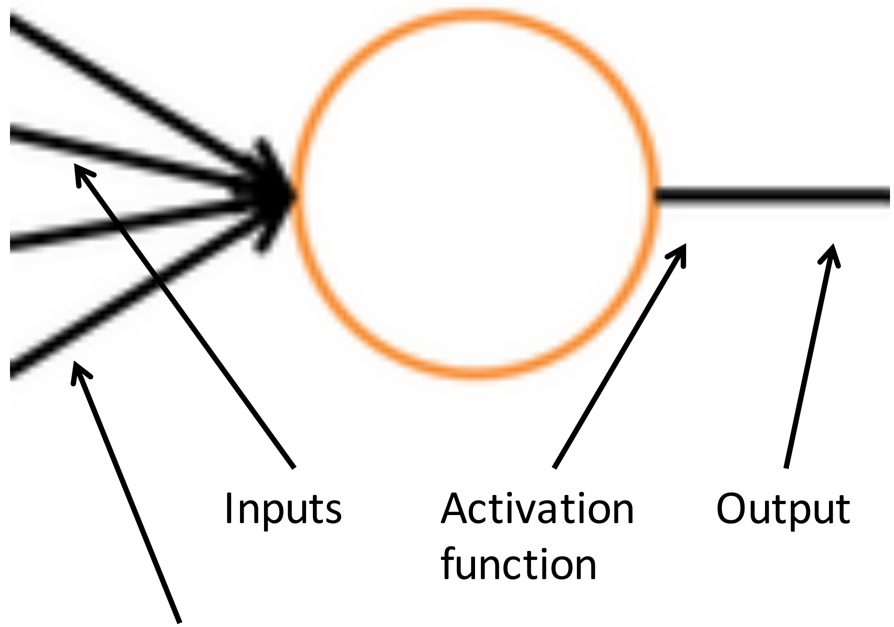
… just like SVMs

But if you understand how softmax models work

Then **you already understand** the operation of a basic neural network neuron!

A single neuron

A computational unit with *n* (3) inputs and 1 output and parameters *W, b*

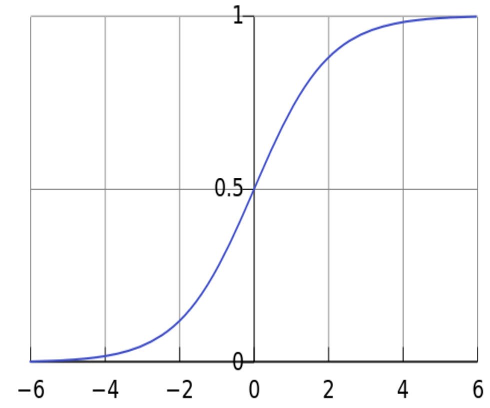


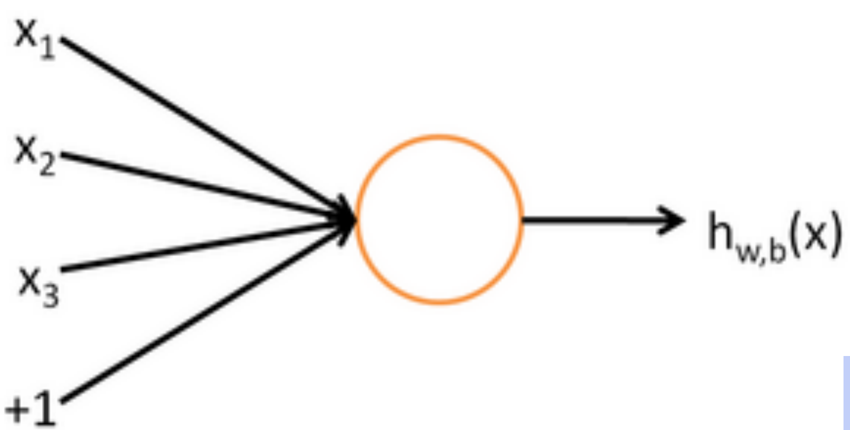
A neuron is essentially a binary logistic regression unit

$$h_{w,b}(x) = f(w^{\mathsf{T}}x + b)$$

b: We can have an "always on" feature, which gives a class prior, or separate it out, as a bias term

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

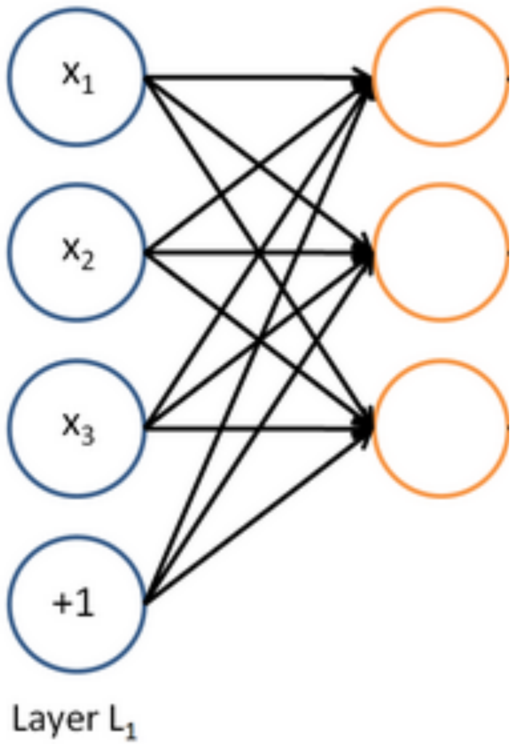




w, *b* are the parameters of this neuron
i.e., this logistic regression model

A neural network
= running several logistic regressions at the same time

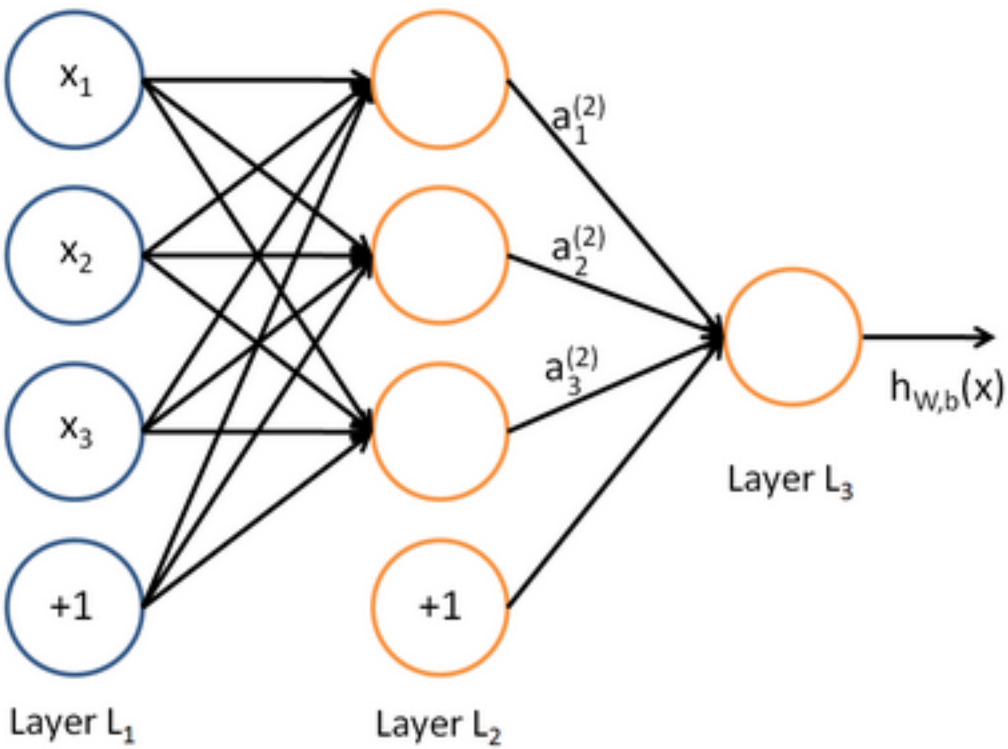
If we feed a vector of inputs through a bunch of logistic regression functions, then we get a vector of outputs …



But we don't have to decide ahead of time what variables these logistic regressions are trying to predict!

A neural network
= running several logistic regressions at the same time

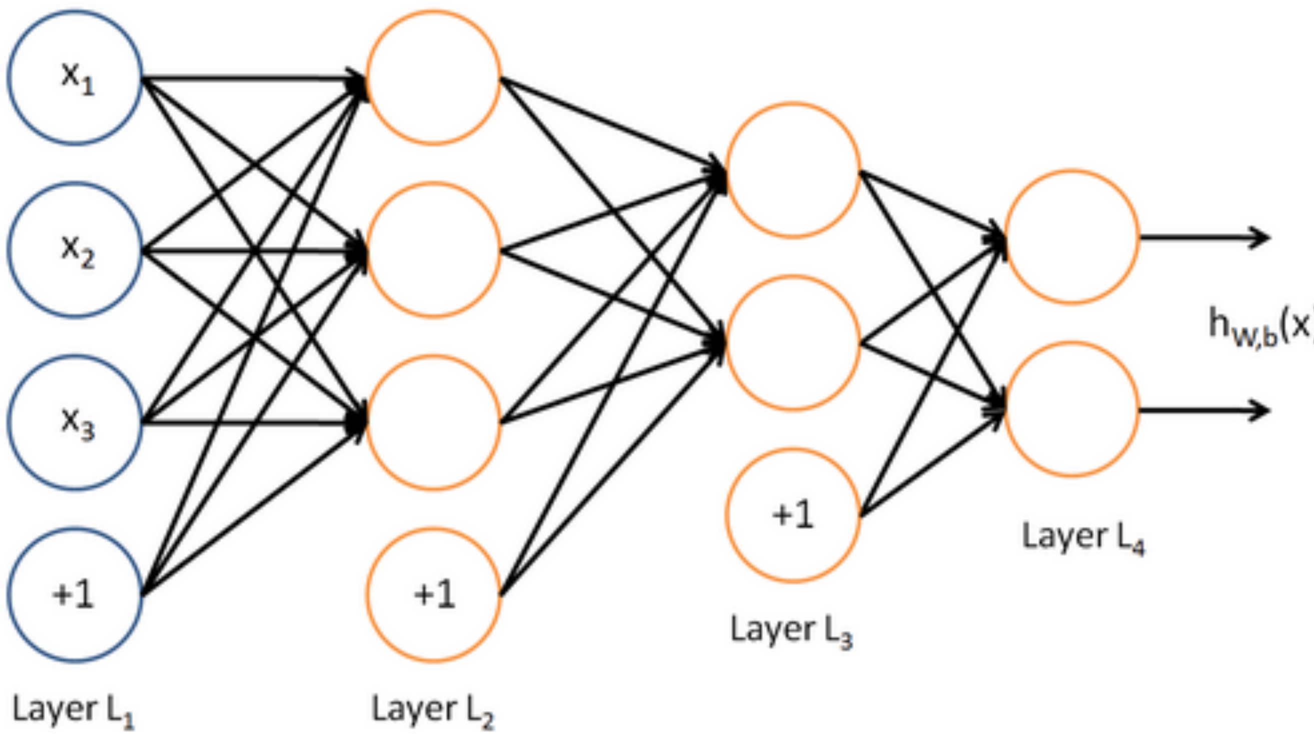
… which we can feed into another logistic regression function



It is the loss function that will direct what the intermediate hidden variables should be, so as to do a good job at predicting the targets for the next layer, etc.

A neural network
= running several logistic regressions at the same time

Before we know it, we have a multilayer neural network….



Matrix notation for a layer

We have

$$a_1 = f(W_{11}x_1 + W_{12}x_2 + W_{13}x_3 + b_1)$$
$$a_2 = f(W_{21}x_1 + W_{22}x_2 + W_{23}x_3 + b_2)$$

etc.

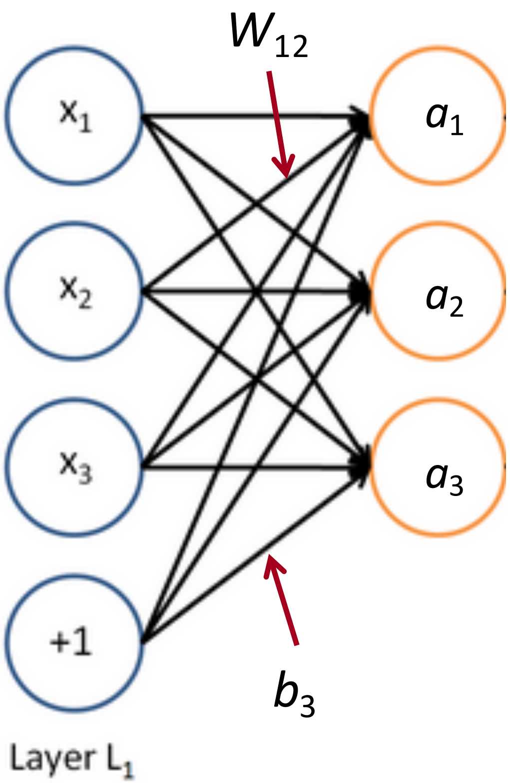
In matrix notation

$$z = Wx + b$$

$$a = f(z)$$

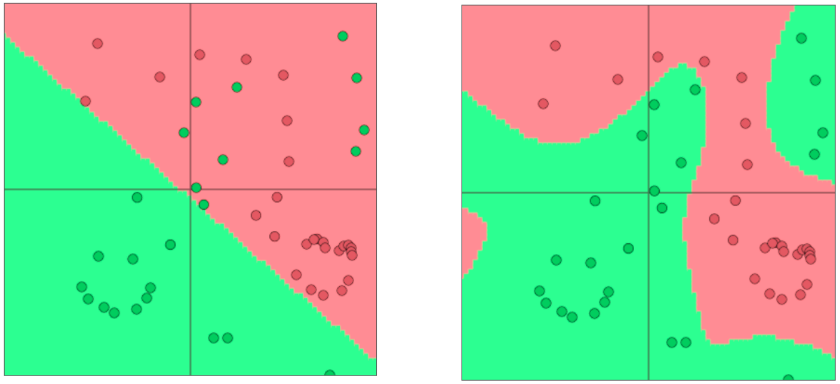
where f is applied element-wise:

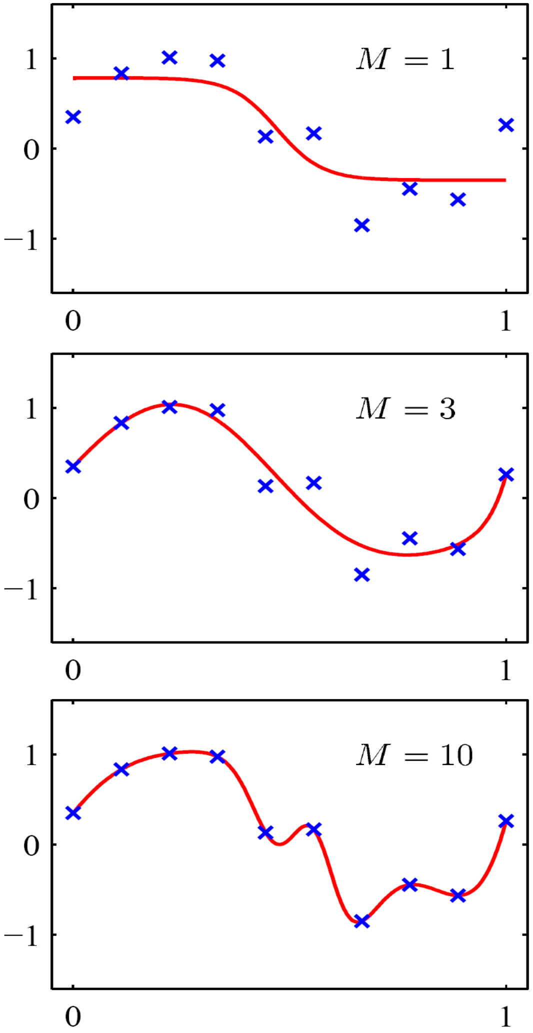
$$f([z_1, z_2, z_3]) = [f(z_1), f(z_2), f(z_3)]$$



Non-linearities (f): Why they're needed

- Example: function approximation, e.g., regression or classification
  - Without non-linearities, deep neural networks can't do anything more than a linear transform
  - Extra layers could just be compiled down into a single linear transform: $W_1 W_2 x = Wx$
  - With more layers, they can approximate more complex functions!





A more powerful window classifier

- Revisiting
- $X_{window} = [\ x_{museums} \quad x_{in} \quad \mathbf{x_{Paris}} \quad x_{are} \quad x_{amazing}\ ]$

A Single Layer Neural Network

- A single layer is a combination of a linear layer and a nonlinearity:

$$\begin{aligned} z &= Wx + b \\ a &= f(z) \end{aligned}$$

- The neural activations *a* can then be used to compute some function
- For instance, a softmax probability or an unnormalized score:

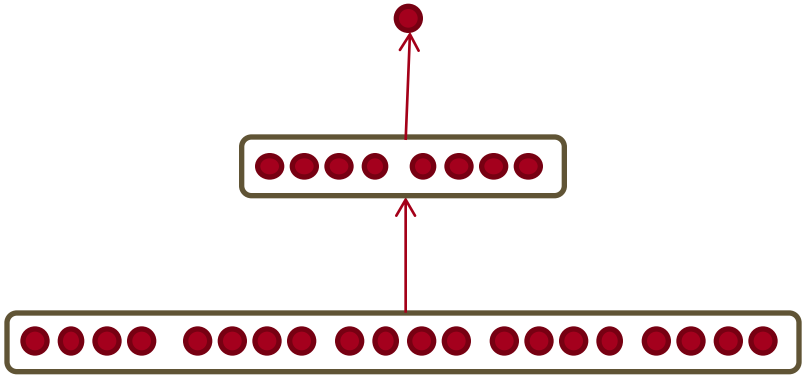
$$score(x) = U^T a \in \mathbb{R}$$

Summary: Feed-forward Computation

Computing a window's score with a 3-layer neural net: *s = score*(museums in Paris are amazing)

$$s = U^T f(Wx + b) \qquad x \in \mathbb{R}^{20\times 1}, W \in \mathbb{R}^{8\times 20}, U \in \mathbb{R}^{8\times 1}$$

$$\begin{aligned} s &= U^T a \\ a &= f(z) \\ z &= Wx + b \end{aligned}$$



X_{window} = [$x_{museums}$ x_{in} x_{Paris} x_{are} $x_{amazing}$]

Next lecture:

Training a window-based neural network.

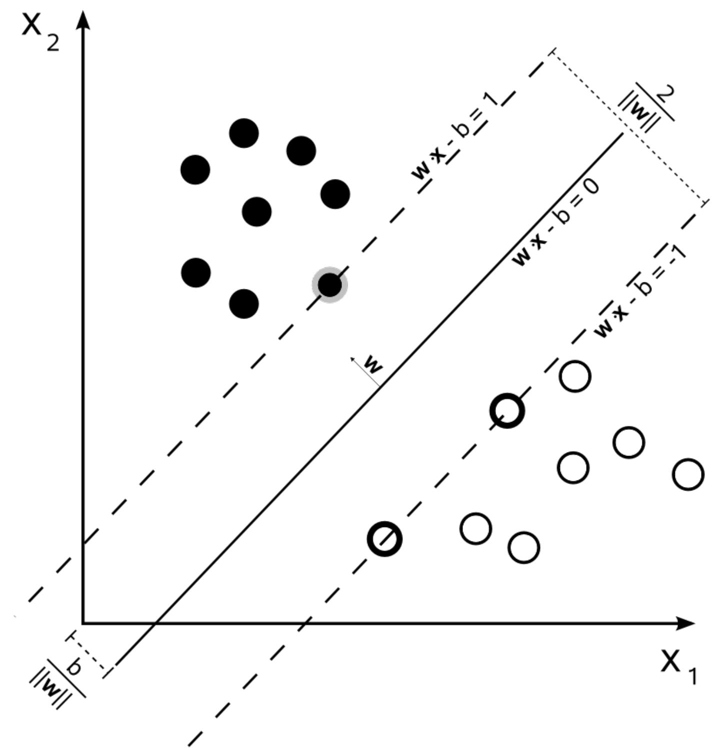
Taking more **deeper derivatives** → **Backprop**

Then we have all the basic tools in place to learn about more complex models :)

Probably for next lecture…

Another output layer and loss function combo!

- So far: softmax and cross-entropy error (exp slow)
- We don't always need probabilities, often unnormalized scores are enough to classify correctly.
- Also: Max-margin!
- More on that in future lectures!



Neural Net model to classify grammatical phrases

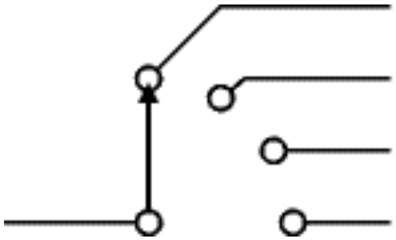
- Idea: Train a neural network to produce high scores for grammatical phrases of specific length and low scores for ungrammatical phrases

- s = score(cat chills on a mat)
- s_c = score(cat chills Menlo a mat)

Another output layer and loss function combo!

- Idea for training objective
- Make score of true window larger and **c**orrupt window's score lower (until they're good enough): minimize

$$J = \max(0, 1 - s + s_c)$$



- This is continuous, can perform SGD

Training with Backpropagation

$$\boxed{J = \max(0, 1 - s + s_c)}$$

$$s = U^T f(Wx + b)$$
$$s_c = U^T f(Wx_c + b)$$

Assuming cost *J* is > 0, it is simple to see that we can compute the derivatives of s and s_c wrt all the involved variables: *U, W, b, x*

$$\frac{\partial s}{\partial U} = \frac{\partial}{\partial U} U^T a \qquad \frac{\partial s}{\partial U} = a$$

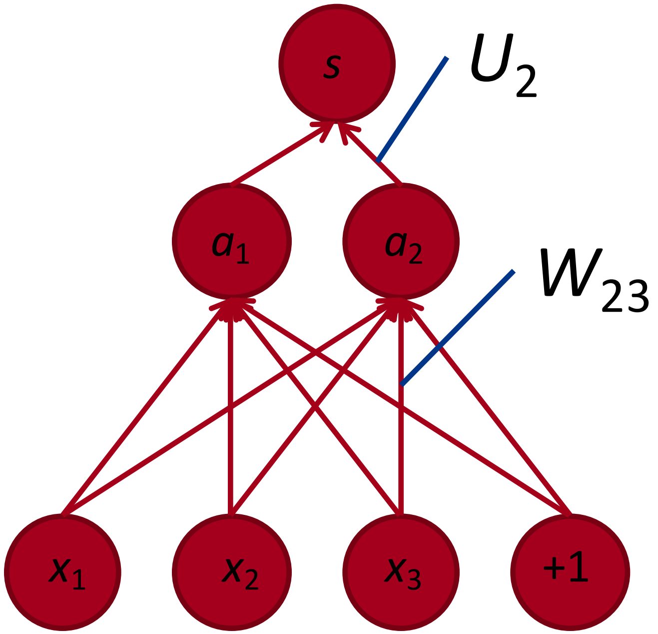
Training with Backpropagation

- Let's consider the derivative of a single weight W_{ij}

$$\frac{\partial s}{\partial W} = \frac{\partial}{\partial W} U^T a = \frac{\partial}{\partial W} U^T f(z) = \frac{\partial}{\partial W} U^T f(Wx + b)$$

- This only appears inside a_i

- For example: W_{23} is only used to compute a_2



Training with Backpropagation

$$\frac{\partial s}{\partial W} = \frac{\partial}{\partial W} U^T a = \frac{\partial}{\partial W} U^T f(z) = \frac{\partial}{\partial W} U^T f(Wx+b)$$

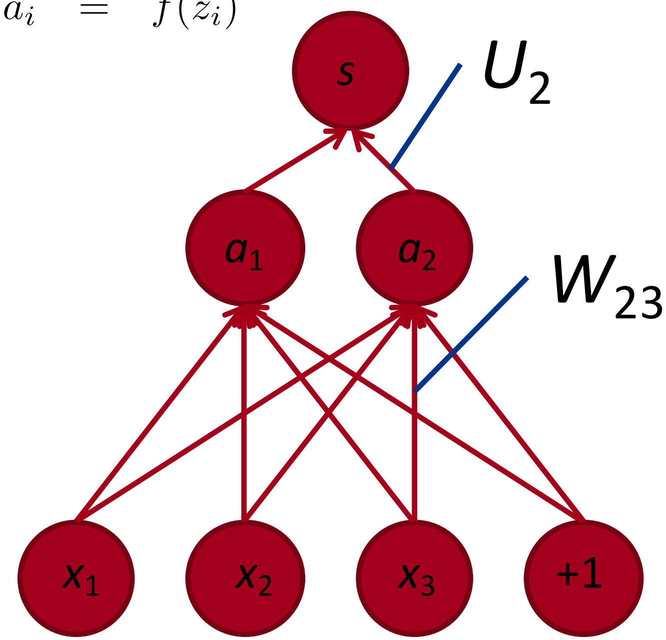
Derivative of weight W_{ij}:

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u}\frac{\partial u}{\partial x}$$

$$\frac{\partial}{\partial W_{ij}} U^T a \quad \rightarrow \quad \frac{\partial}{\partial W_{ij}} U_i a_i$$

$$\begin{aligned} z_i &= W_{i\cdot}x + b_i = \sum_{j=1}^{3} W_{ij}x_j + b_i \\ a_i &= f(z_i) \end{aligned}$$

$$\begin{aligned} U_i \frac{\partial}{\partial W_{ij}} a_i &= U_i \frac{\partial a_i}{\partial z_i} \frac{\partial z_i}{\partial W_{ij}} \\ &= U_i \frac{\partial f(z_i)}{\partial z_i} \frac{\partial z_i}{\partial W_{ij}} \\ &= U_i f'(z_i) \frac{\partial z_i}{\partial W_{ij}} \\ &= U_i f'(z_i) \frac{\partial W_{i\cdot}x + b_i}{\partial W_{ij}} \end{aligned}$$



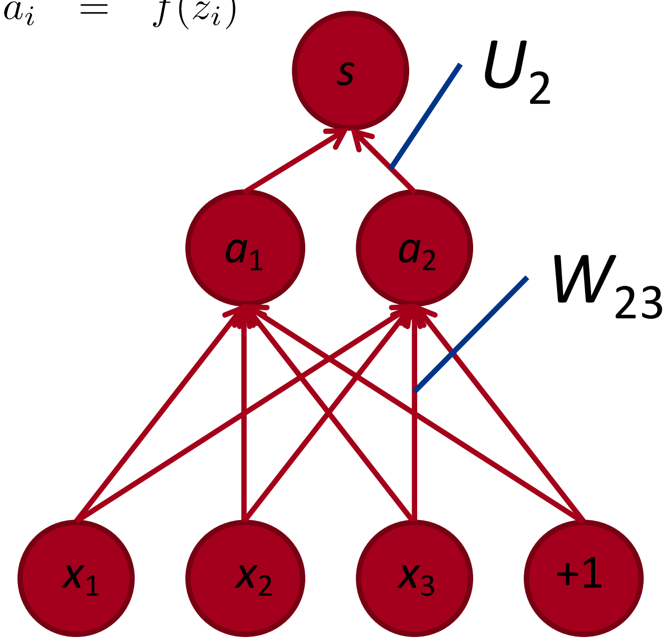
Training with Backpropagation

Derivative of single weight W_{ij} :

$$U_i \frac{\partial}{\partial W_{ij}} a_i$$

$$
\begin{aligned}
&= U_i f'(z_i) \frac{\partial W_{i\cdot} x + b_i}{\partial W_{ij}} \\
&= U_i f'(z_i) \frac{\partial}{\partial W_{ij}} \sum_k W_{ik} x_k \\
&= \underbrace{U_i f'(z_i)} x_j \\
&= \underbrace{\delta_i}_{\text{Local error signal}} \; \underbrace{x_j}_{\text{Local input signal}}
\end{aligned}
$$

$$
\begin{aligned}
z_i &= W_{i\cdot} x + b_i = \sum_{j=1}^{3} W_{ij} x_j + b_i \\
a_i &= f(z_i)
\end{aligned}
$$



where $f'(z) = f(z)(1 - f(z))$ for logistic f

Training with Backpropagation

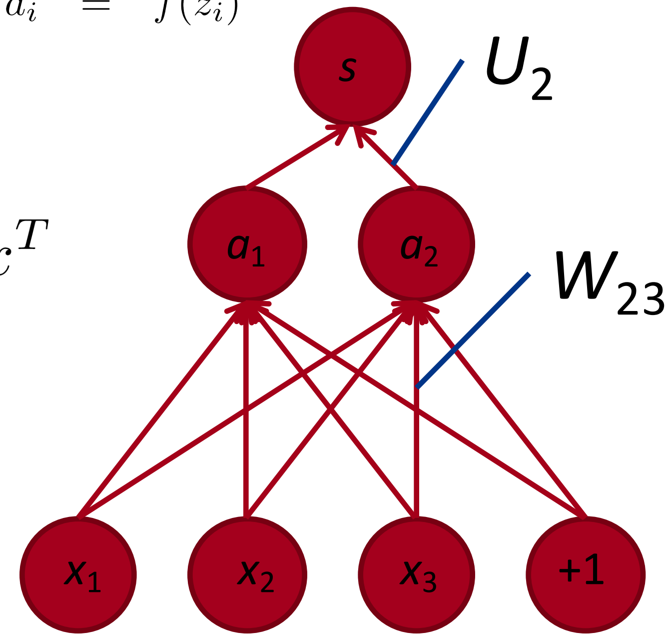
- From single weight W_{ij} to full W:

$$\frac{\partial J}{\partial W_{ij}} = \underbrace{U_i f'(z_i)}_{\delta_i} x_j = \delta_i \quad x_j$$

$$z_i = W_{i\cdot}x + b_i = \sum_{j=1}^{3} W_{ij}x_j + b_i$$

$$a_i = f(z_i)$$

- We want all combinations of $i = 1, 2$ and $j = 1, 2, 3$
- Solution: Outer product: $\frac{\partial J}{\partial W} = \delta x^T$ where $\delta \in \mathbb{R}^{2\times 1}$ is the "responsibility" coming from each activation a

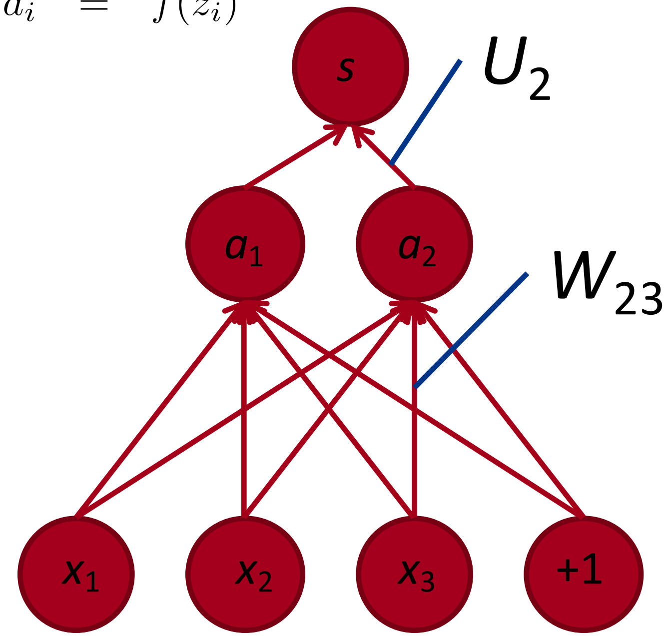


Training with Backpropagation

- For biases *b*, we get:

$$
\begin{aligned}
& U_i \frac{\partial}{\partial b_i} a_i \\
= \quad & U_i f'(z_i) \frac{\partial W_i . x + b_i}{\partial b_i} \\
= \quad & \delta_i
\end{aligned}
$$

$$
\begin{aligned}
z_i &= W_i . x + b_i = \sum_{j=1}^{3} W_{ij} x_j + b_i \\
a_i &= f(z_i)
\end{aligned}
$$



Training with Backpropagation

That's almost backpropagation

It's simply taking derivatives and using the chain rule!

Remaining trick: we can re-use derivatives computed for higher layers in computing derivatives for lower layers

Example: last derivatives of model, the word vectors in *x*

Training with Backpropagation

- Take derivative of score with respect to single word vector (for simplicity a 1d vector, but same if it was longer)
- Now, we cannot just take into consideration one a_i because each x_j is connected to all the neurons above and hence x_j influences the overall score through all of these, hence:

$$
\begin{aligned}
\frac{\partial s}{\partial x_j} &= \sum_{i=1}^{2} \frac{\partial s}{\partial a_i} \frac{\partial a_i}{\partial x_j} \\
&= \sum_{i=1}^{2} \frac{\partial U^T a}{\partial a_i} \frac{\partial a_i}{\partial x_j} \\
&= \sum_{i=1}^{2} U_i \frac{\partial f(W_{i\cdot}x + b)}{\partial x_j} \\
&= \sum_{i=1}^{2} \underbrace{U_i f'(W_{i\cdot}x + b)} \frac{\partial W_{i\cdot}x}{\partial x_j} \\
&= \sum_{i=1}^{2} \delta_i W_{ij} \\
&= \underbrace{\delta^T}_{\text{Re-used part of previous derivative}} W_{\cdot j}
\end{aligned}
$$

Summary