Computation Graphs & Backpropagation

CMSC 723 / LING 723 / INST 725

Hal Daumé III [he/him]

12 Sep 2019

(Many slides c/o Marine Carpuat)

Announcements, logistics

- HW1 is done!
- HW2:
  - Written portion will be posted in the next 24 hours
  - Programming portion will be posted before next class (hopefully earlier)

- Question: do you find the recorded class videos useful?

Today

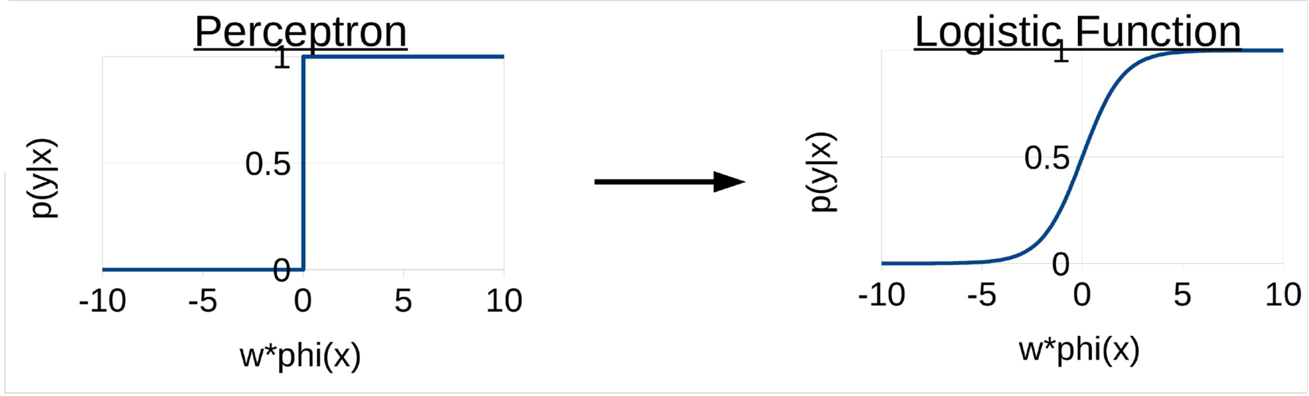
- Quick refresher on logistic regression
- Extension to non-linear models
  - aka neural networks
  - aka deep learning
  - aka artificial intelligence!!!!

- Framing: Much of NLP is about good
  - input representations
  - output representations
  - how to connect them

Logistic Regression review

The logistic function

$$P(y=1|x)=\frac{e^{\mathbf{w}\cdot\boldsymbol{\varphi}(x)}}{1+e^{\mathbf{w}\cdot\boldsymbol{\varphi}(x)}}$$



- x: the input
- **φ(x)**: vector of feature functions $\{\varphi_1(x), \varphi_2(x), \ldots, \varphi_I(x)\}$
- **w**: the weight vector $\{w_1, w_2, \ldots, w_I\}$
- y: the prediction, +1 if “yes”, -1 if “no”

- Can account for uncertainty
- Differentiable

Logistic regression: how to train?

- Train based on **conditional likelihood**
- Find parameters w that maximize conditional likelihood of all answers y_i given examples x_i

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmax}} \prod_i P(y_i | x_i ; \mathbf{w})$$

Stochastic gradient ascent (or descent)

- Online training algorithm for logistic regression
  - and other probabilistic models

```
create map w
for I iterations
    for each labeled pair x, y in the data
        w += α * dP(y|x)/dw
```

- Update weights for every training example
- Move in direction given by gradient
- Size of update step scaled by learning rate

Gradient of the logistic function

$$
\begin{aligned}
\frac{d}{dw} P(y=1|x) &= \frac{d}{dw} \frac{e^{w\cdot\varphi(x)}}{1+e^{w\cdot\varphi(x)}} \\
&= \varphi(x) \frac{e^{w\cdot\varphi(x)}}{\left(1+e^{w\cdot\varphi(x)}\right)^2}
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dw} P(y=-1|x) &= \frac{d}{dw} \left(1 - \frac{e^{w\cdot\varphi(x)}}{1+e^{w\cdot\varphi(x)}}\right) \\
&= -\varphi(x) \frac{e^{w\cdot\varphi(x)}}{\left(1+e^{w\cdot\varphi(x)}\right)^2}
\end{aligned}
$$

Example: Person/not-person classification problem

Given an introductory sentence in Wikipedia

predict whether the article is about a person

Given	Predict
Gonso was a Sanron sect priest (754-827) in the late Nara and early Heian periods.	Yes!
Shichikuzan Chigogataki Fudomyoo is a historical site located at Magura, Maizuru City, Kyoto Prefecture.	No!

Example: initial update

- Set α=1, initialize **w=0**

x = A site , located in Maizuru , Kyoto   y = -1

$$\boldsymbol{w}\cdot\varphi(x)=0 \qquad \frac{d}{dw}P(y=-1|x) = -\frac{e^0}{(1+e^0)^2}\varphi(x)$$

$$= -0.25\varphi(x)$$

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + -0.25\varphi(x)$$

$w_{\text{unigram "Maizuru"}}$ = -0.25
$w_{\text{unigram ","}}$ = -0.5
$w_{\text{unigram "in"}}$ = -0.25
$w_{\text{unigram "Kyoto"}}$ = -0.25
$w_{\text{unigram "A"}}$ = -0.25
$w_{\text{unigram "site"}}$ = -0.25
$w_{\text{unigram "located"}}$ = -0.25

Example: second update

$\mathbf{x}$ = Shoken , monk born in Kyoto $\quad\quad y = 1$

-0.5 $\quad$ -0.25 $\quad$ -0.25

$$\mathbf{w}\cdot\varphi(x) = -1 \qquad \frac{d}{d\,\mathbf{w}} P(y=1|x) = \frac{e^{1}}{(1+e^{1})^{2}}\varphi(x)$$

$$= 0.196\,\varphi(x)$$

$$\mathbf{w} \leftarrow \mathbf{w} + 0.196\,\varphi(x)$$

$w_{\text{unigram “Maizuru”}}$	= -0.25	$w_{\text{unigram “A”}}$	= -0.25	$w_{\text{unigram “Shoken”}}$	= 0.196
$w_{\text{unigram “,”}}$	= -0.304	$w_{\text{unigram “site”}}$	= -0.25	$w_{\text{unigram “monk”}}$	= 0.196
$w_{\text{unigram “in”}}$	= -0.054	$w_{\text{unigram “located”}}$	= -0.25	$w_{\text{unigram “born”}}$	= 0.196
$w_{\text{unigram “Kyoto”}}$	= -0.054				

Multiclass version

$$\mathrm{p}(y \mid \boldsymbol{x}) = \frac{\exp\left(\boldsymbol{\theta}^\top \boldsymbol{f}(\boldsymbol{x}, y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{f}(\boldsymbol{x}, y')\right)}.$$

Some models are better then others…

- Consider these 2 examples

-1	he saw a bird in the park
+1	he saw a robbery in the park

- Which of the 2 models below is better?

Classifier 1	Classifier 2
he +3	bird -1
saw -5	robbery +1
a +0.5	
bird -1	
robbery +1	
in +5	
the -3	
park -2	

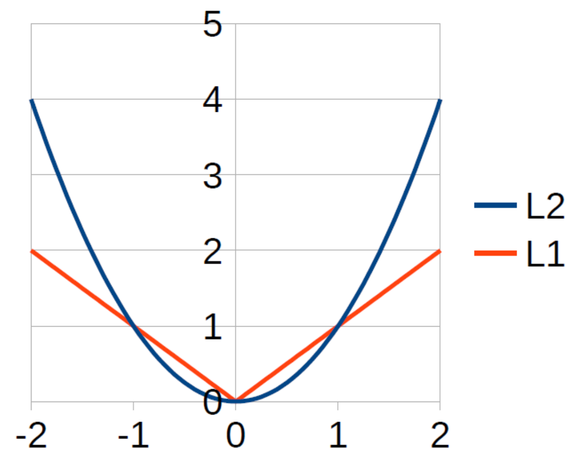
Classifier 2 will probably generalize better!
It does not include irrelevant information
=> Smaller model is better

Regularization

- A penalty on adding extra weights

- L2 regularization: $\|w\|_2$
  - big penalty on large weights
  - small penalty on small weights

- L1 regularization: $\|w\|_1$
  - Uniform increase when large or small
  - Will cause many weights to become zero



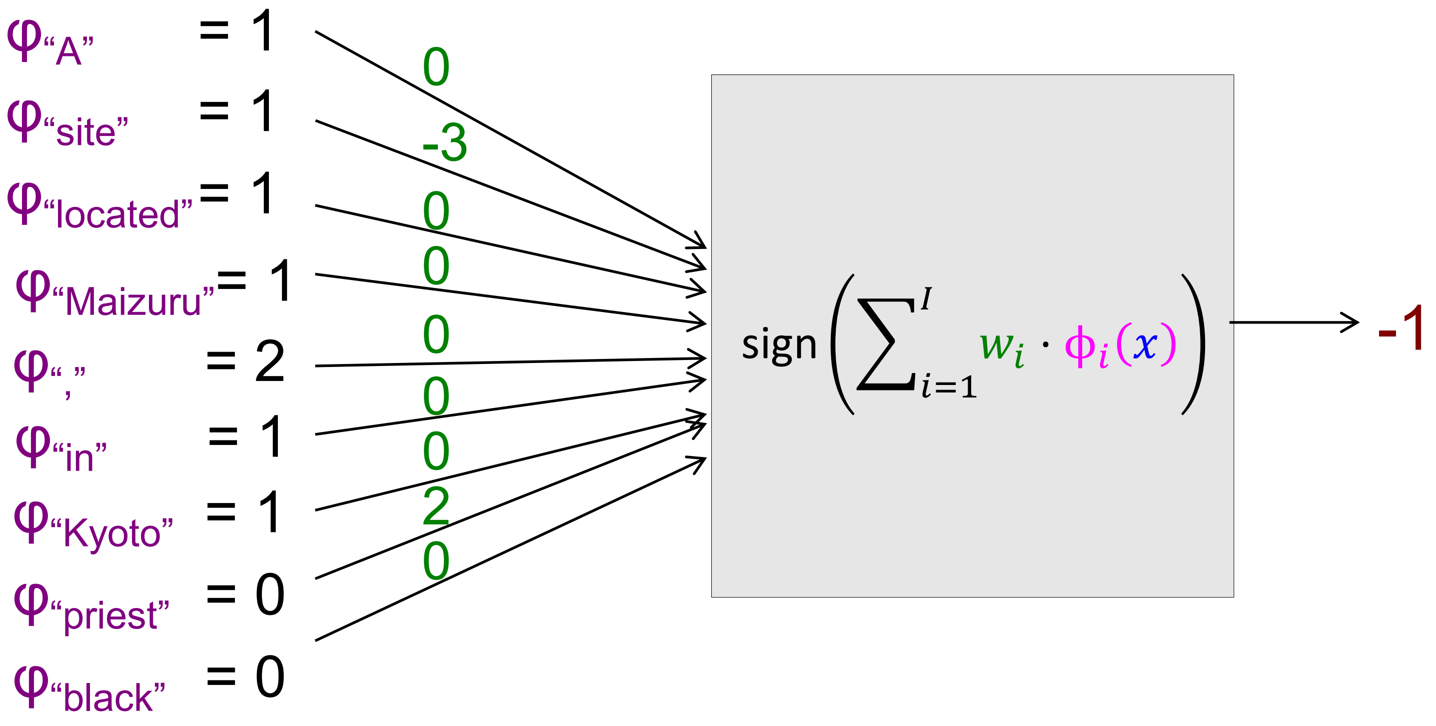
Neural networks

Formalizing binary prediction

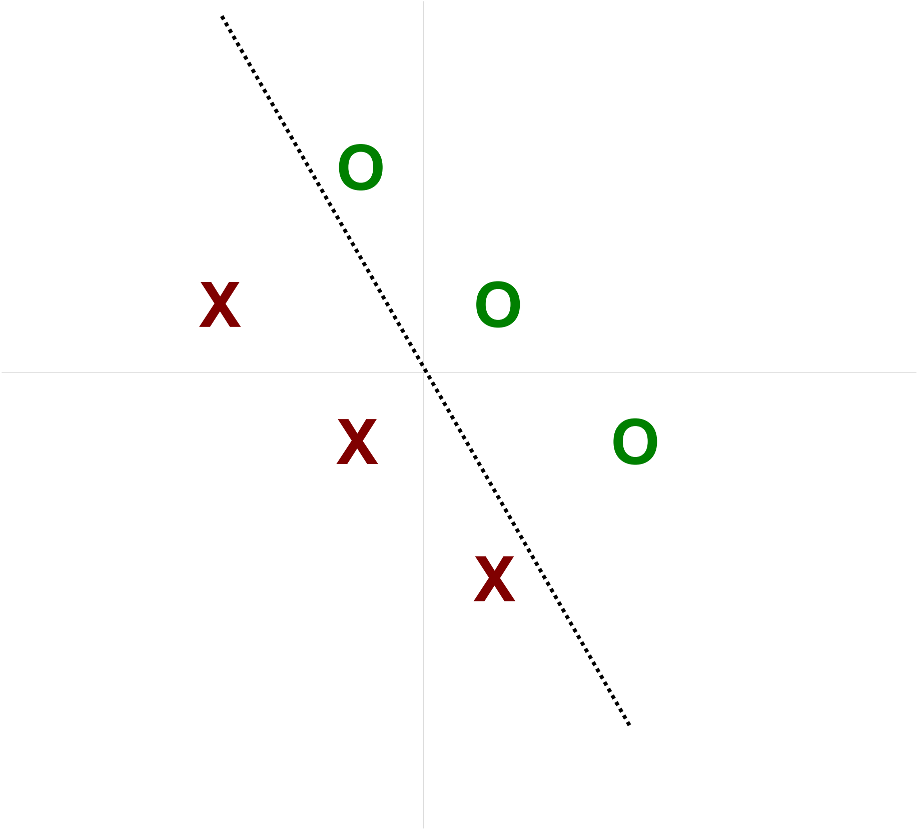
$$
\begin{aligned}
y &= \operatorname{sign}\left(\mathbf{w} \cdot \boldsymbol{\varphi}(x)\right) \\
&= \operatorname{sign}\left(\sum_{i=1}^{I} w_i \cdot \varphi_i(x)\right)
\end{aligned}
$$

- x: the input
- **φ(x)**: vector of feature functions $\{\varphi_1(x), \varphi_2(x), \ldots, \varphi_I(x)\}$
- **w**: the weight vector $\{w_1, w_2, \ldots, w_I\}$
- y: the prediction, +1 if "yes", -1 if "no"
    - (sign(v) is +1 if v >= 0, -1 otherwise)

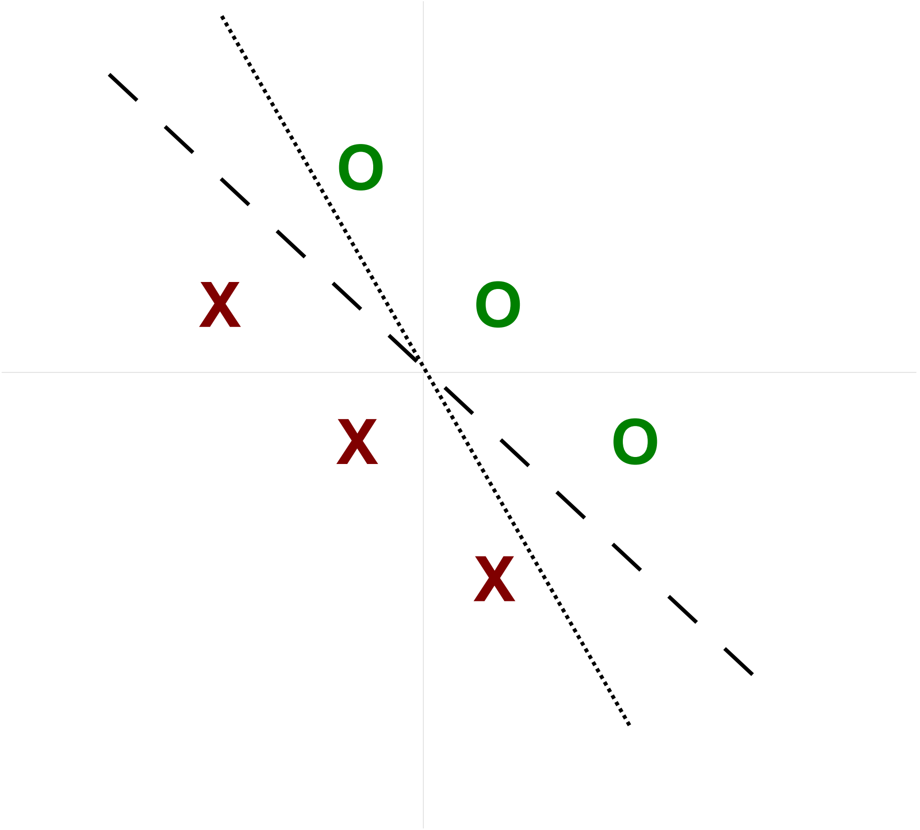
Linear models:
a "machine" to calculate a weighted sum



Linear models : Geometric interpretation

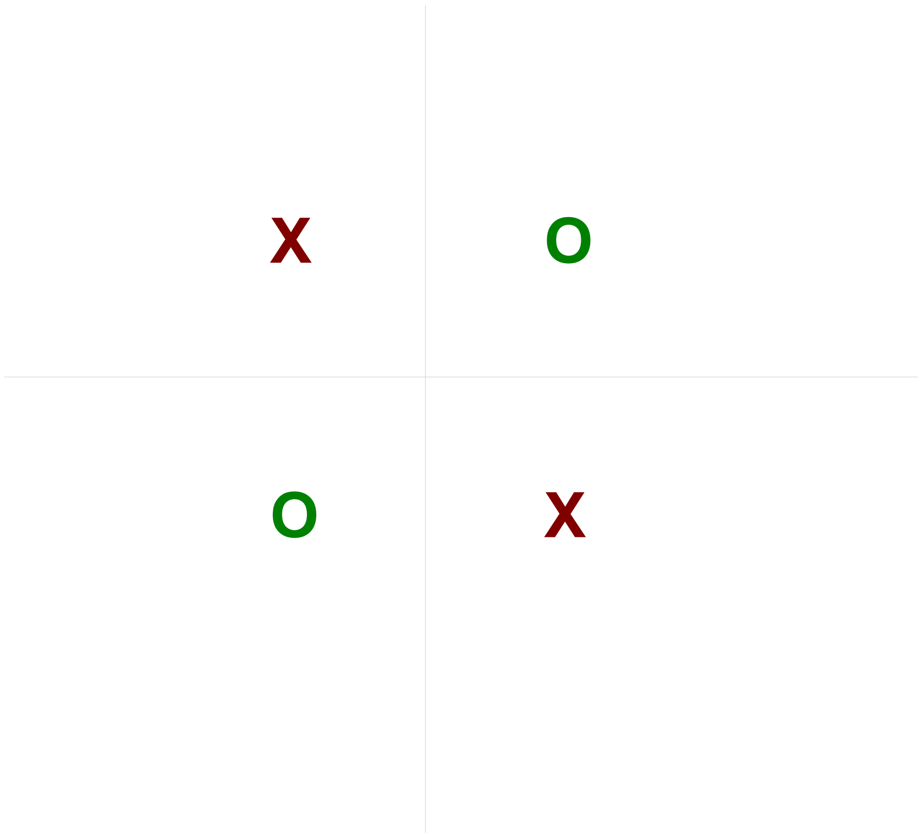


Linear models :
Geometric interpretation



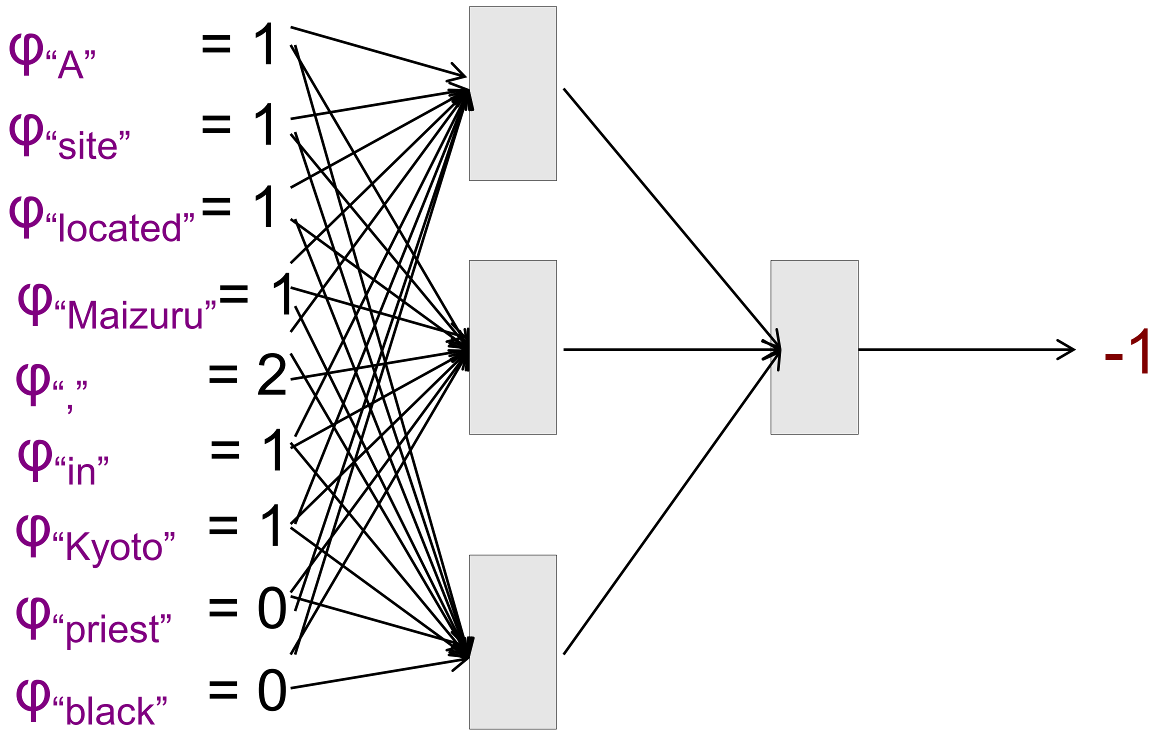
Limitation of linear models

- can only find **linear separations** between positive and negative examples



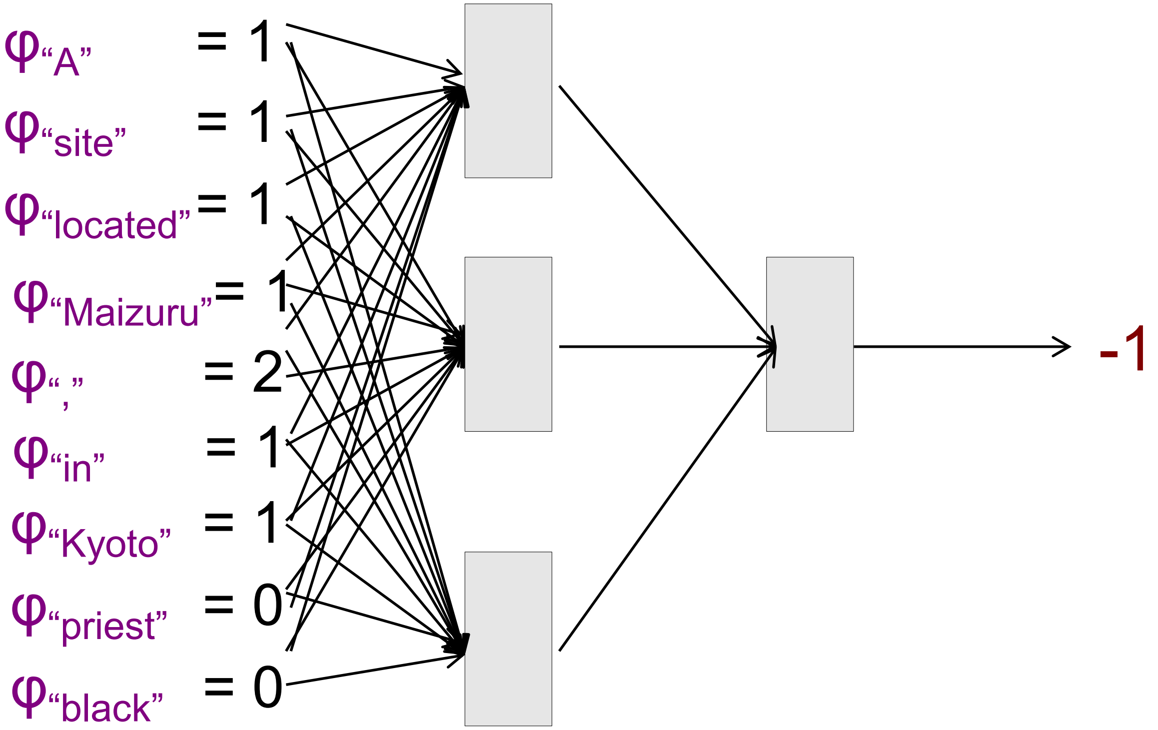
Neural Networks

- Connect together multiple linear models with non-linear “activations”



- Motivation: Can represent non-linear functions!

Neural Networks: key terms



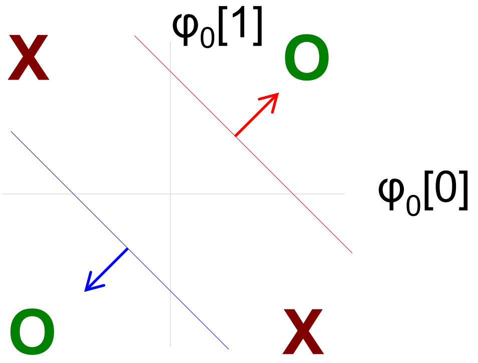
- Input (aka features)
- Output
- Nodes
- Layers
- Hidden layers
- Activation function (non-linear)

- Multi-layer perceptron

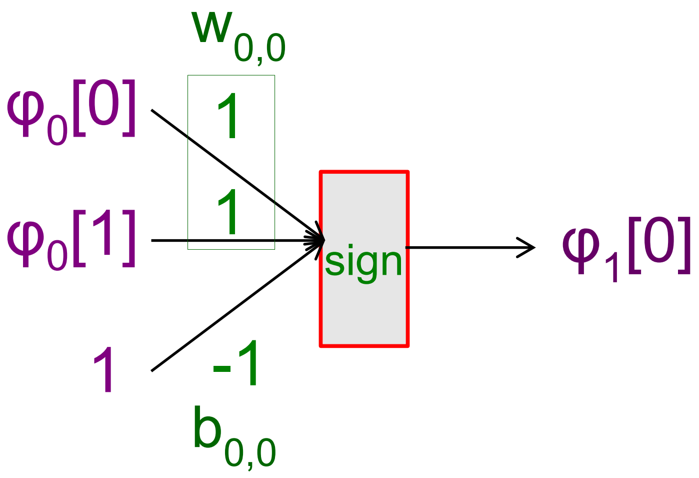
Example

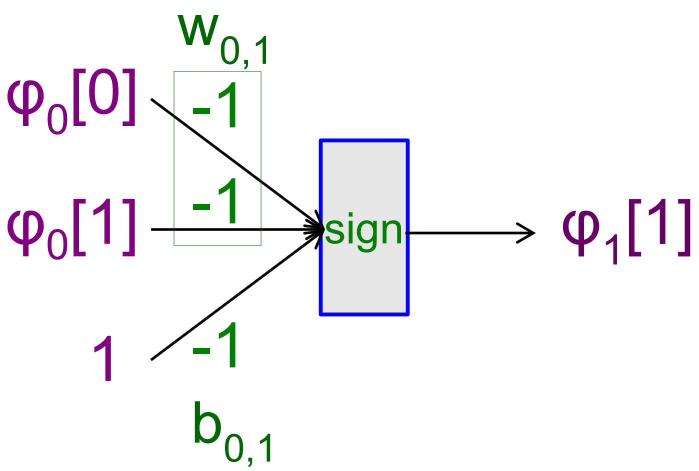
- Create two classifiers

$\varphi_0(x_1) = \{-1, 1\}$ $\varphi_0(x_2) = \{1, 1\}$



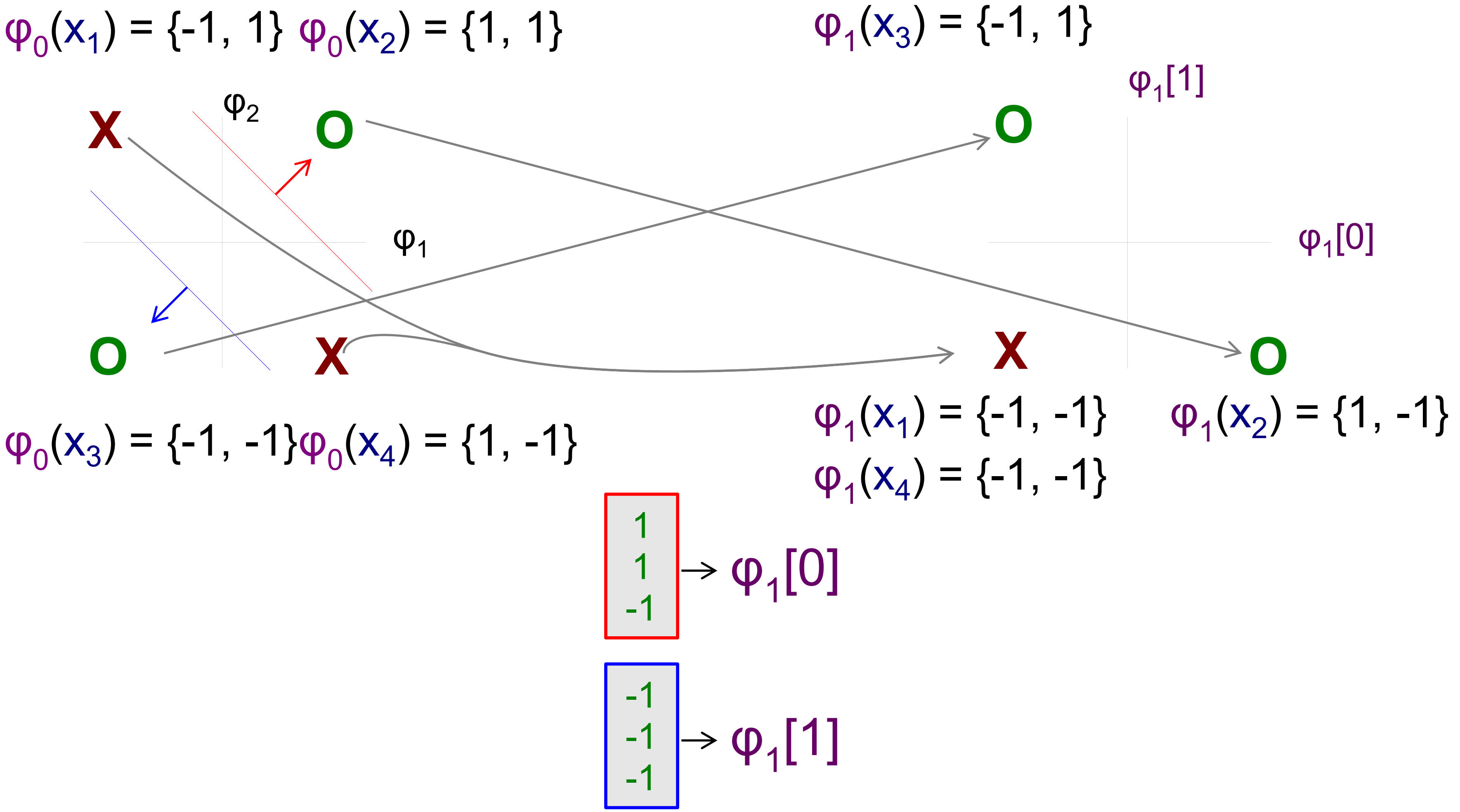
$\varphi_0(x_3) = \{-1, -1\}$ $\varphi_0(x_4) = \{1, -1\}$





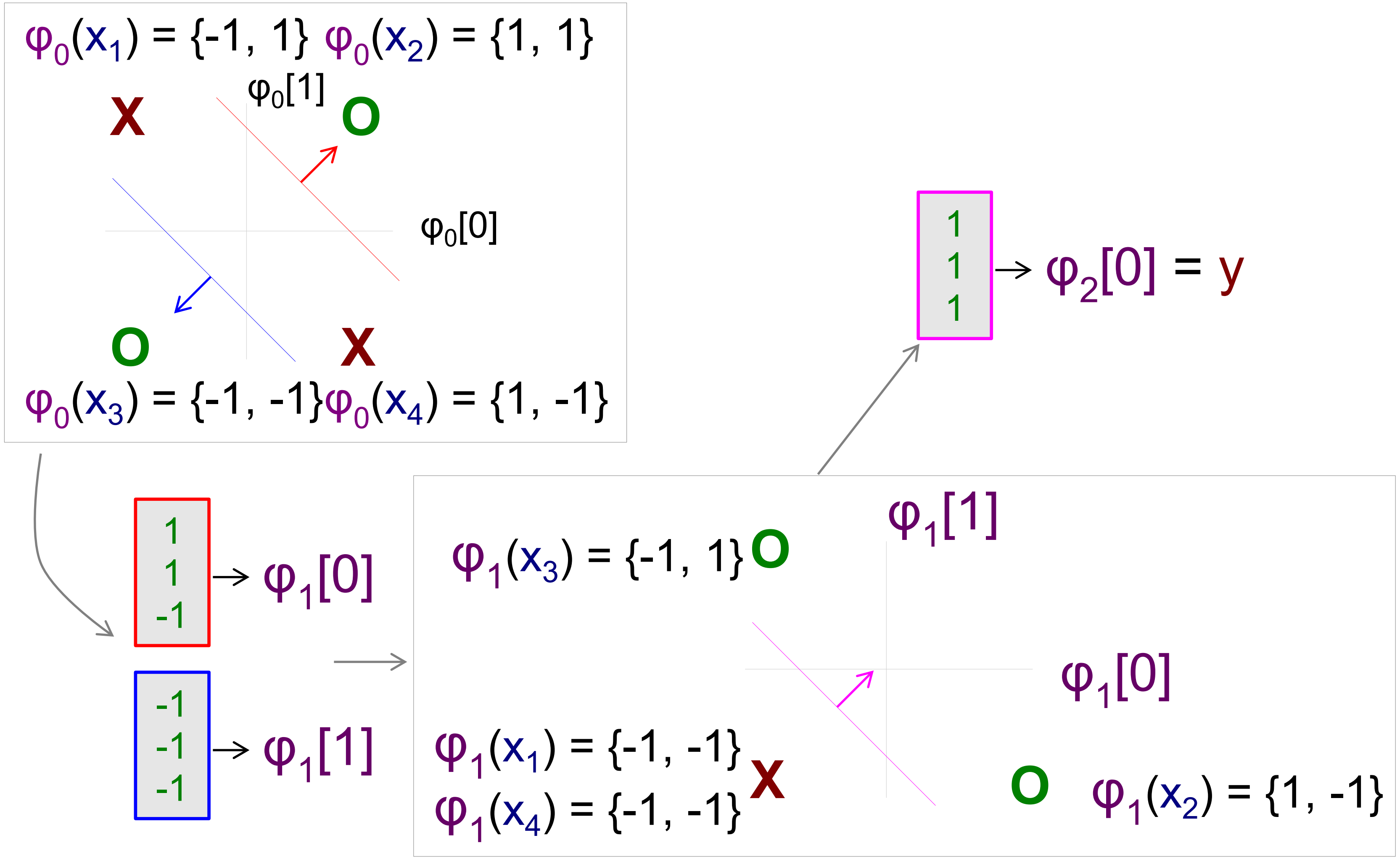
Example

- These classifiers map to a new space



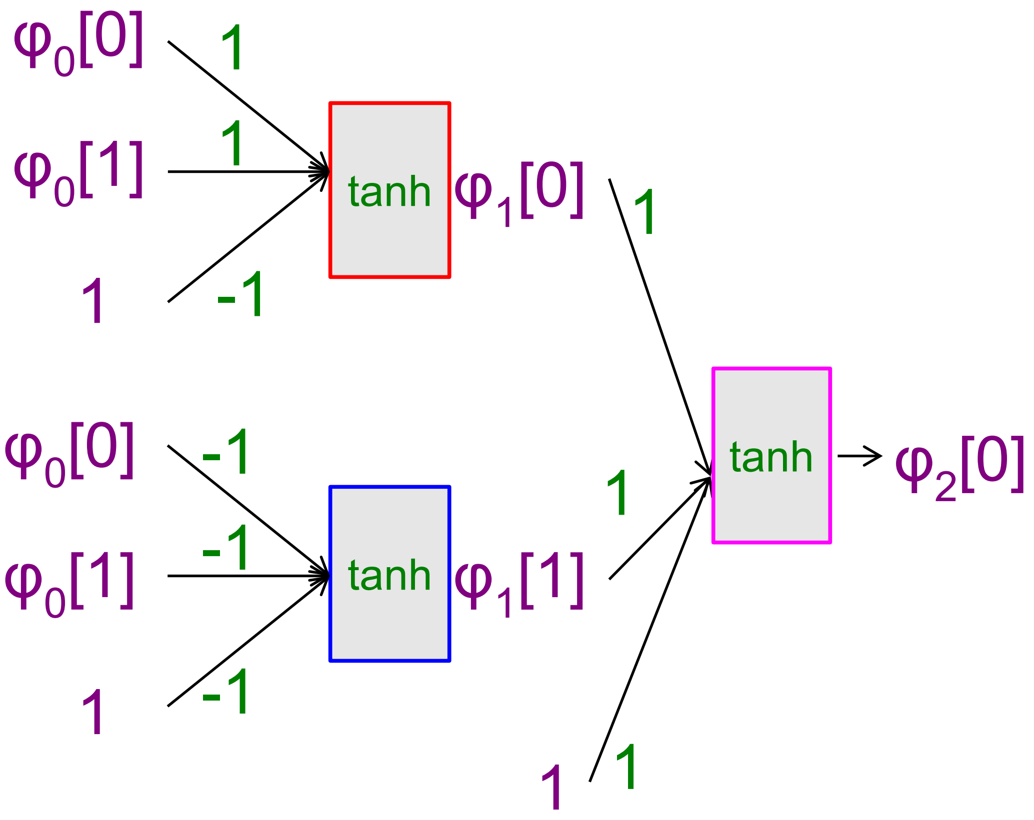
Example

- In new space, the examples are linearly separable!



Example wrap-up: Forward propagation

- The final net



Softmax Function for multiclass classification

- Sigmoid function for multiple classes

$$P(y \mid x) = \frac{e^{\mathbf{w}\cdot\phi(x,y)}}{\sum_{\tilde{y}} e^{\mathbf{w}\cdot\phi(x,\tilde{y})}}$$

Current class

Sum of other classes

- Can be expressed using matrix/vector ops

$$\mathbf{r} = \exp\left(\mathbf{W}\cdot\phi(x,y)\right)$$

$$\mathbf{p} = \mathbf{r}/\sum_{\tilde{r}\in\mathbf{r}}\tilde{r}$$

Stochastic Gradient Descent

Online training algorithm for probabilistic models

$w = \mathbf{0}$
for *I* iterations
  for each labeled pair *x, y* in the data
    $w \mathrel{+}= \alpha * dP(y|x)/dw$

In other words

- For every training example, calculate the gradient (the direction that will increase the probability of y)
- Move in that direction, multiplied by learning rate α

Gradient of the Sigmoid Function

Take the derivative of the probability

$$\frac{d}{dw}P(y=1\mid x) = \frac{d}{dw}\frac{e^{\mathbf{w}\cdot\phi(x)}}{1+e^{\mathbf{w}\cdot\phi(x)}}$$

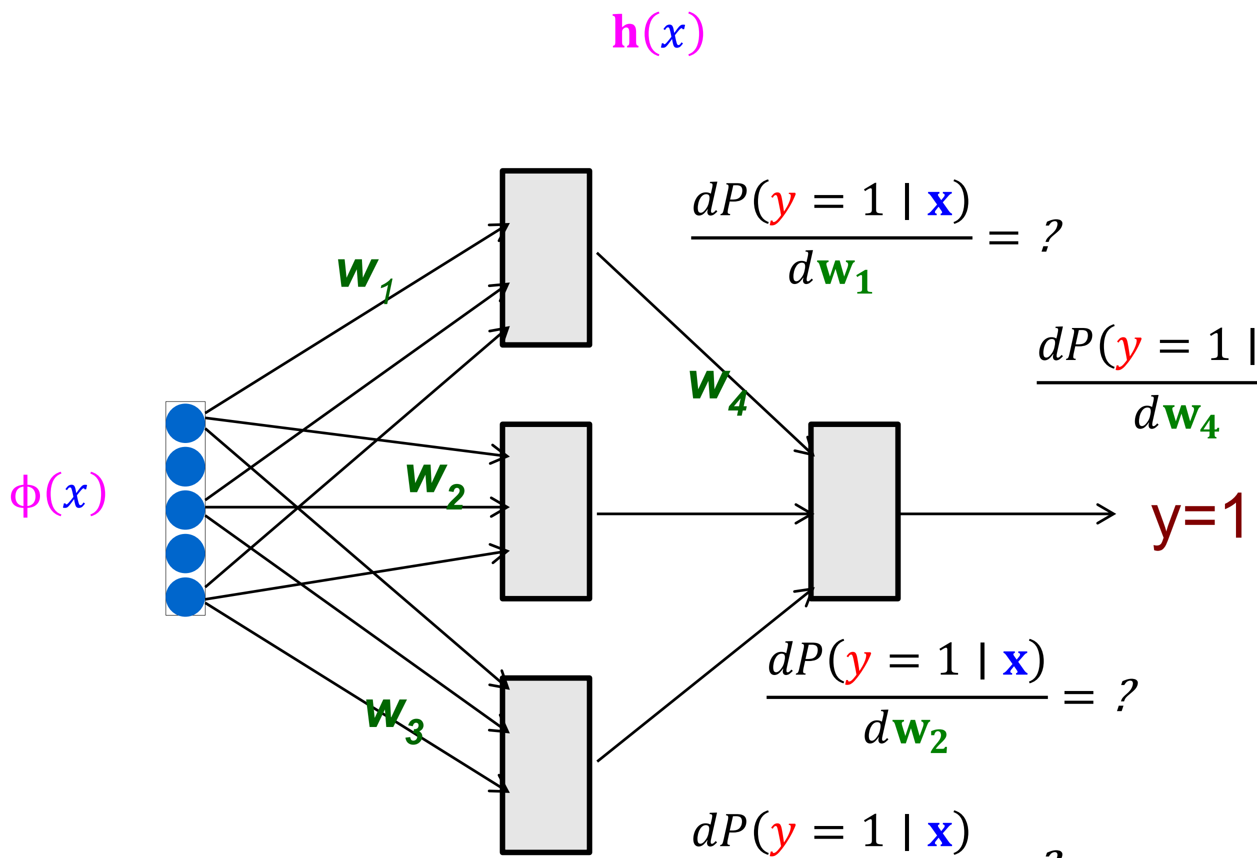
$$= \phi(x)\frac{e^{\mathbf{w}\cdot\phi(x)}}{(1+e^{\mathbf{w}\cdot\phi(x)})^2}$$

$$\frac{d}{dw}P(y=-1\mid x) = \frac{d}{dw}\left(1-\frac{e^{\mathbf{w}\cdot\phi(x)}}{1+e^{\mathbf{w}\cdot\phi(x)}}\right)$$

$$= -\phi(x)\frac{e^{\mathbf{w}\cdot\phi(x)}}{(1+e^{\mathbf{w}\cdot\phi(x)})^2}$$

Learning: We Don't Know the Derivative for Hidden Units!

For NNs, only know correct tag for last layer



$$\frac{dP(y=1 \mid \mathbf{x})}{d\mathbf{w_1}} = ?$$

$$\frac{dP(y=1 \mid \mathbf{x})}{d\mathbf{w_4}} = \mathbf{h}(x) \frac{e^{\mathbf{w_4} \cdot \mathbf{h}(x)}}{(1+e^{\mathbf{w_4} \cdot \mathbf{h}(x)})^2}$$

$$\frac{dP(y=1 \mid \mathbf{x})}{d\mathbf{w_2}} = ?$$

$$\frac{dP(y=1 \mid \mathbf{x})}{d\mathbf{w_3}} = ?$$

Answer: Back-Propagation

Calculate derivative with chain rule

$$\frac{dP(y=1\mid x)}{d\mathbf{w_1}} = \frac{dP(y=1\mid x)}{d\mathbf{w_4}\mathbf{h}(\mathbf{x})}\frac{d\mathbf{w_4}\mathbf{h}(\mathbf{x})}{dh_1(\mathbf{x})}\frac{dh_1(\mathbf{x})}{d\mathbf{w_1}}$$

$$\frac{e^{\mathbf{w_4}\cdot\mathbf{h}(x)}}{(1+e^{\mathbf{w_4}\cdot\mathbf{h}(x)})^2} \qquad w_{1,4}$$

Error of next unit (δ_4)

Weight

Gradient of this unit

In General

Calculate *i* based on next units *j*:

$$\frac{dP(y=1\mid \mathbf{x})}{\mathbf{w_i}} = \frac{dh_i(\mathbf{x})}{d\mathbf{w_i}}\sum_j \delta_j\, w_{i,j}$$

Backpropagation

=

Gradient descent

+

Chain rule

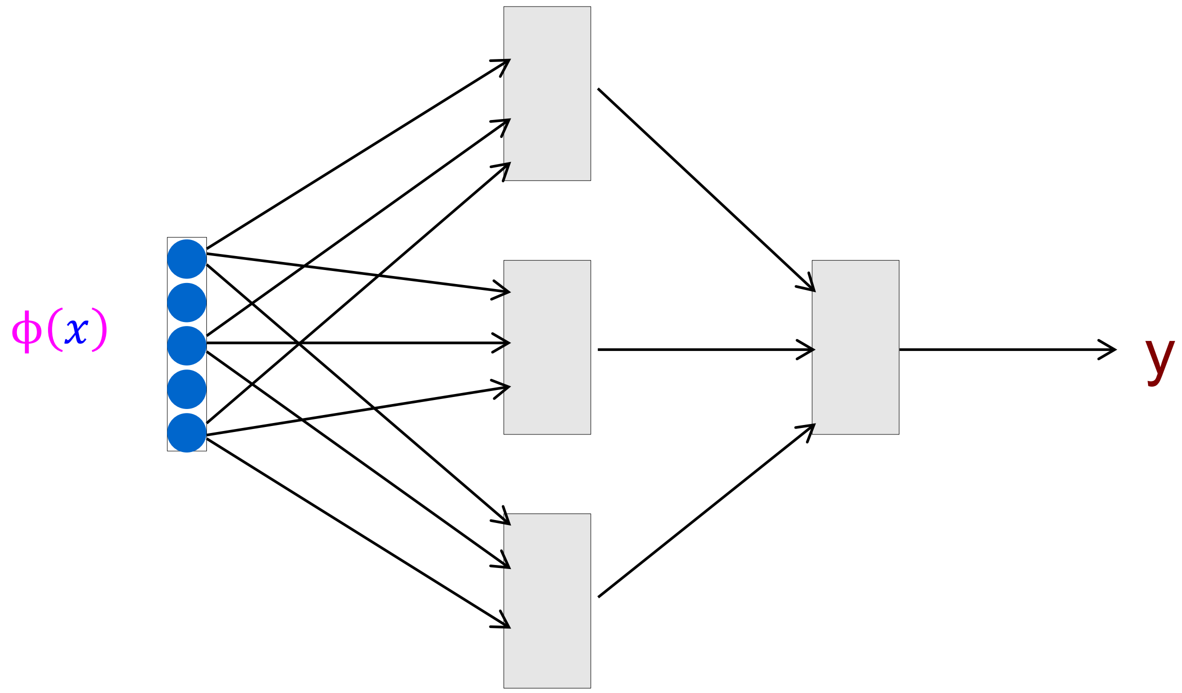
Note: for the mathematically inclined, this is "not quite true."

For details on why, see Tim Vieira's nice blog post:

timvieira.github.io/blog/post/2017/08/18/backprop-is-not-just-the-chain-rule

Feed Forward Neural Nets

All connections point **forward**



It is a directed acyclic graph (DAG)

Neural Networks summary

- Non-linear classification
- Prediction: forward propagation
  - Vector/matrix operations + non-linearities
- Training: backpropagation + stochastic gradient descent

For more details, see [CIML Chap 7]