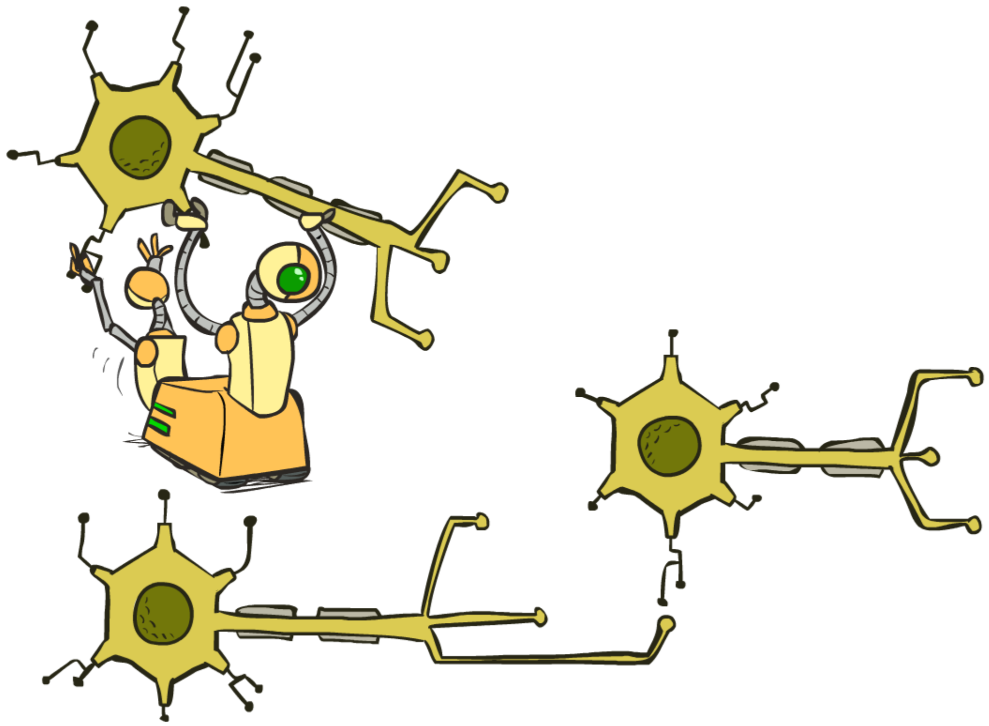
Announcements

- Gradescope
  - You must assign questions to page numbers when you submit so the TAs can easily find your answers.
  - You will get a 0 otherwise!
- HW4 due today!
- P2 due on Thursday!
- Midterm next week!

CS 188: Artificial Intelligence

Optimization and Neural Nets

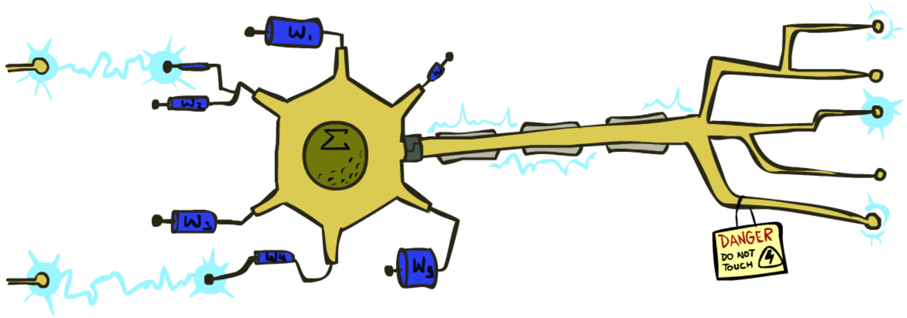


Instructor: Anca Dragan --- University of California, Berkeley

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

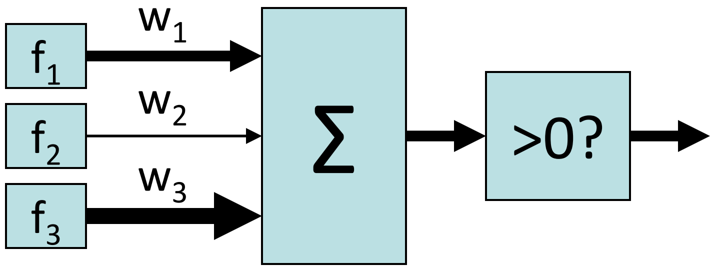
Reminder: Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation



$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

- If the activation is:
  - Positive, output +1
  - Negative, output -1



Feature Vectors

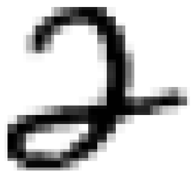
x $f(x)$ y

```
Hello,

Do you want free printr
cartriges?  Why pay more
when you can get them
ABSOLUTELY FREE!  Just
```

```
# free       : 2
YOUR_NAME    : 0
MISSPELLED   : 2
FROM_FRIEND  : 0
...
```

SPAM or Not SPAM



```
PIXEL-7,12   : 1
PIXEL-7,13   : 0
...
NUM_LOOPS    : 1
...
```

“2”

Feature Vectors

x | $f(x)$ | y

```
Hello,

Do you want free printr
cartriges?  Why pay more
when you can get them
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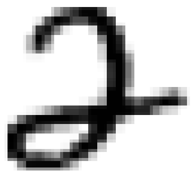
SPAM or Not SPAM



```
PIXEL-7,12   : 1
PIXEL-7,13   : 0
...
NUM_LOOPS    : 1
...
```

“2”

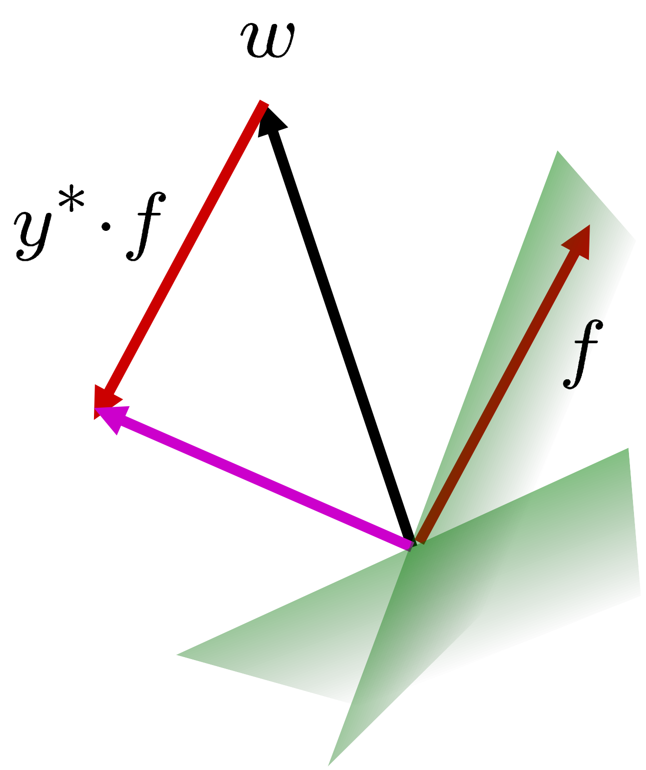
Learning: Binary Perceptron

- Start with weights = 0
- For each training instance:
  - Classify with current weights

$$y = \begin{cases} +1 & \text{if } w \cdot f(x) \geq 0 \\ -1 & \text{if } w \cdot f(x) < 0 \end{cases}$$

  - If correct (i.e., y=y*), no change!
  - If wrong: adjust the weight vector by adding or subtracting the feature vector. Subtract if y* is -1.

$$w = w + y^* \cdot f$$



Before update $w^T f(x) > 0$ and $y^* = -1$

After update

$$(w - f(x))^T f(x) = w^T f(x) - f(x)^T f(x) < w^T f(x)$$

Multiclass Decision Rule

- If we have multiple classes:
  - A weight vector for each class:

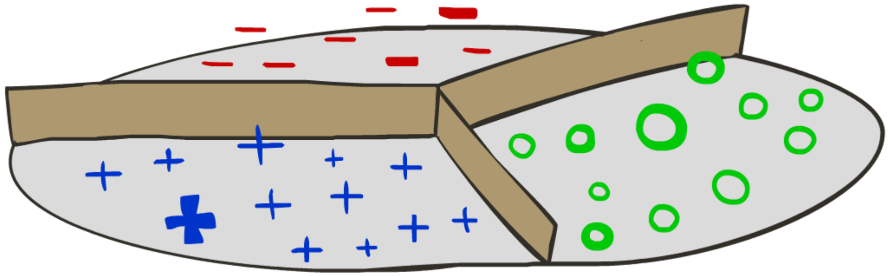
    $$w_y$$

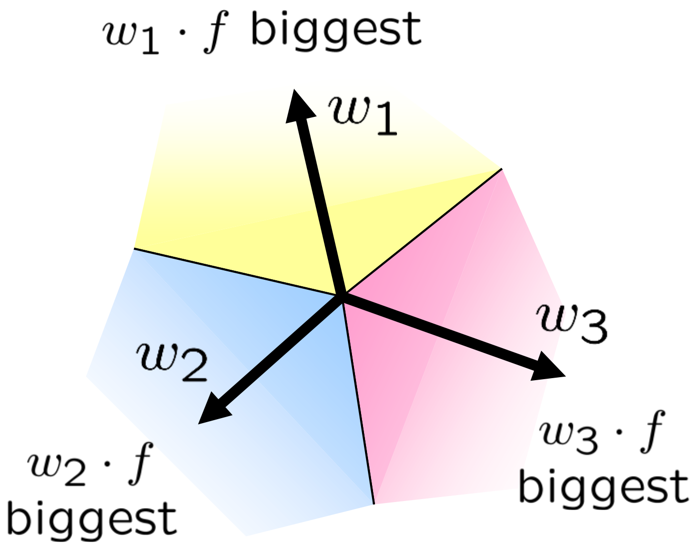
  - Score (activation) of a class y:

    $$w_y \cdot f(x)$$

  - Prediction highest score wins

    $$y = \arg\max_y \; w_y \cdot f(x)$$





Binary = multiclass where the negative class has weight zero

Learning: Multiclass Perceptron

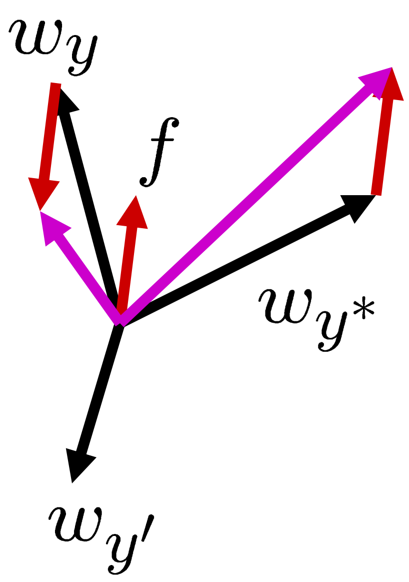
- Start with all weights = 0
- Pick up training examples one by one
- Predict with current weights

$$y = \arg\max_y \; w_y \cdot f(x)$$

- If correct, no change!
- If wrong: lower score of wrong answer, raise score of right answer

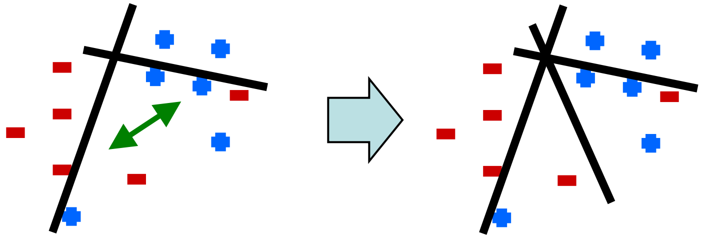
$$w_y = w_y - f(x)$$

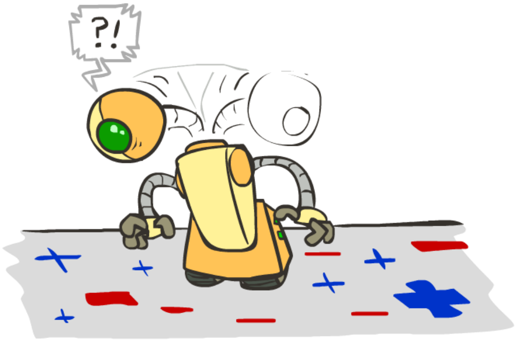
$$w_{y^*} = w_{y^*} + f(x)$$



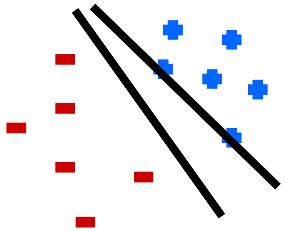
Problems with the Perceptron

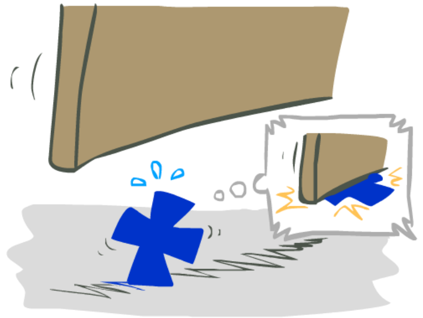
- Noise: if the data isn't separable, weights might thrash
  - Averaging weight vectors over time can help (averaged perceptron)



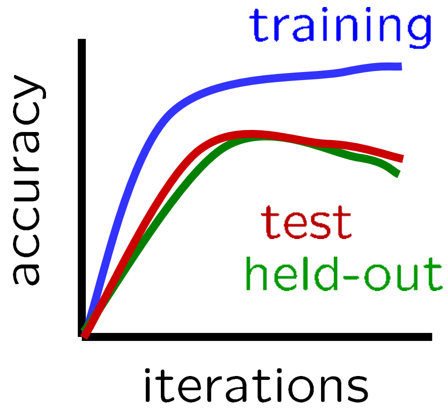


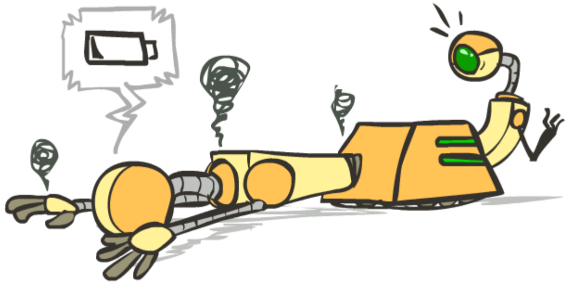
- Mediocre generalization: finds a "barely" separating solution



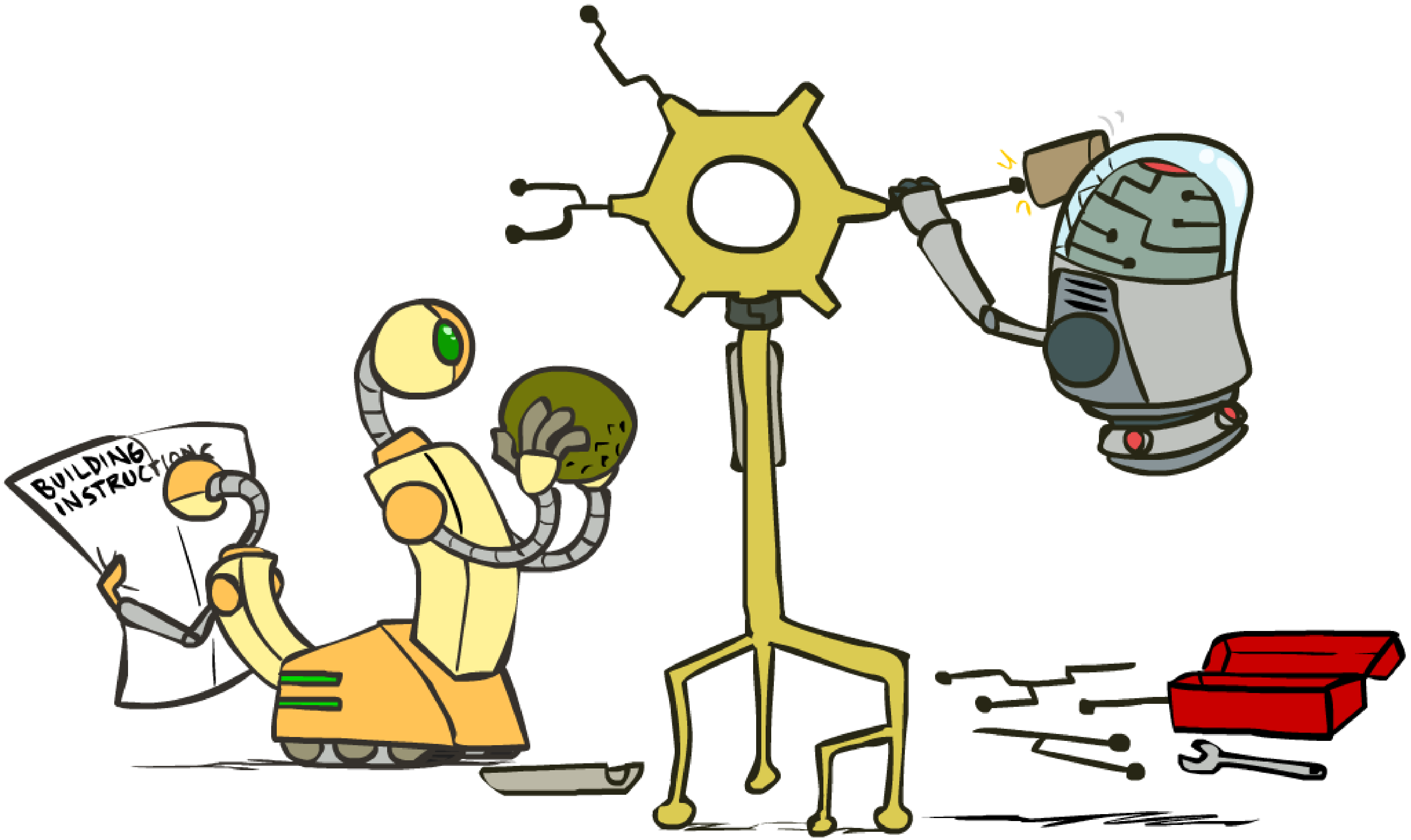


- Overtraining: test / held-out accuracy usually rises, then falls
  - Overtraining is a kind of overfitting

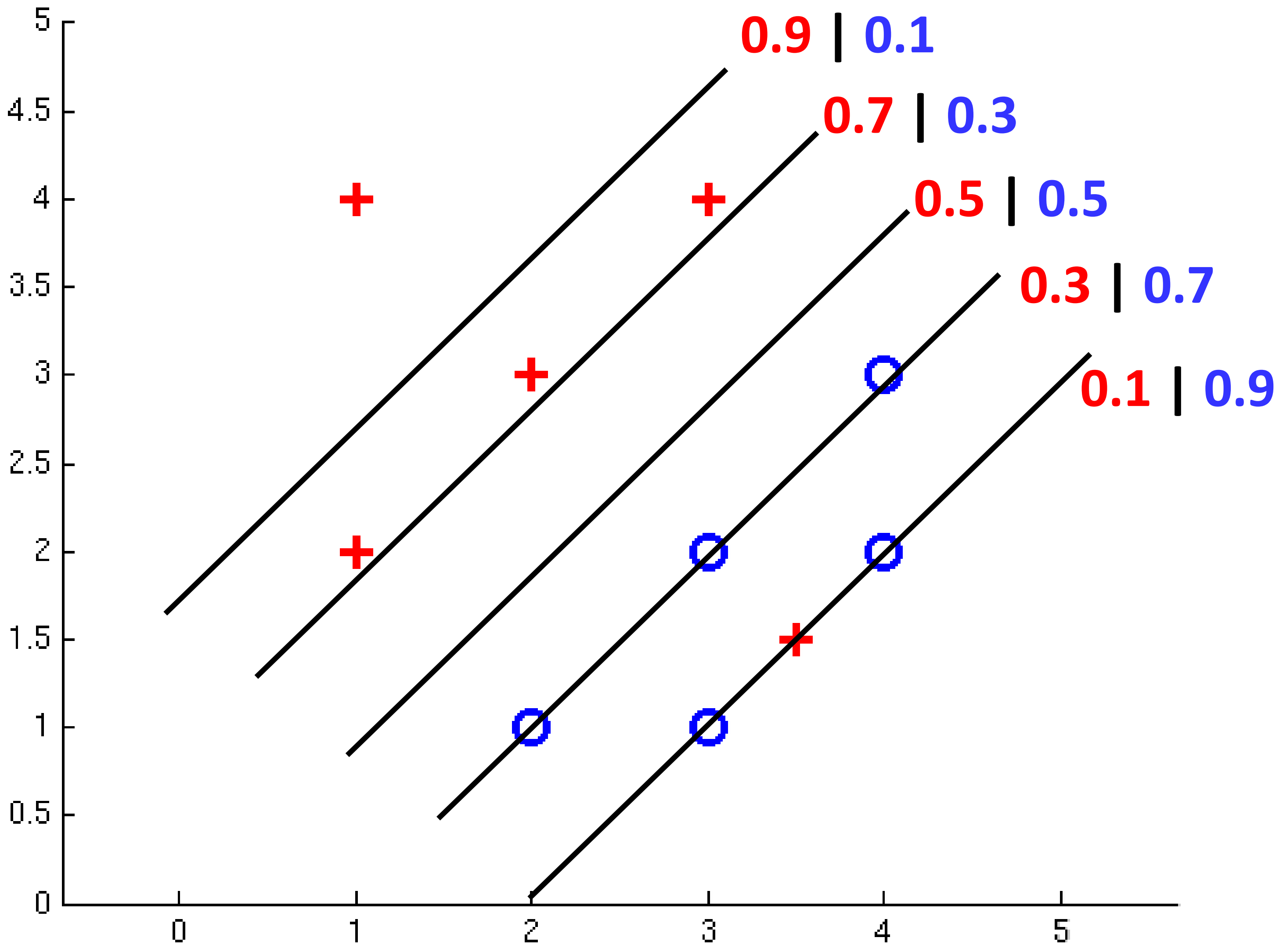




Improving the Perceptron



Non-Separable Case: Probabilistic Decision

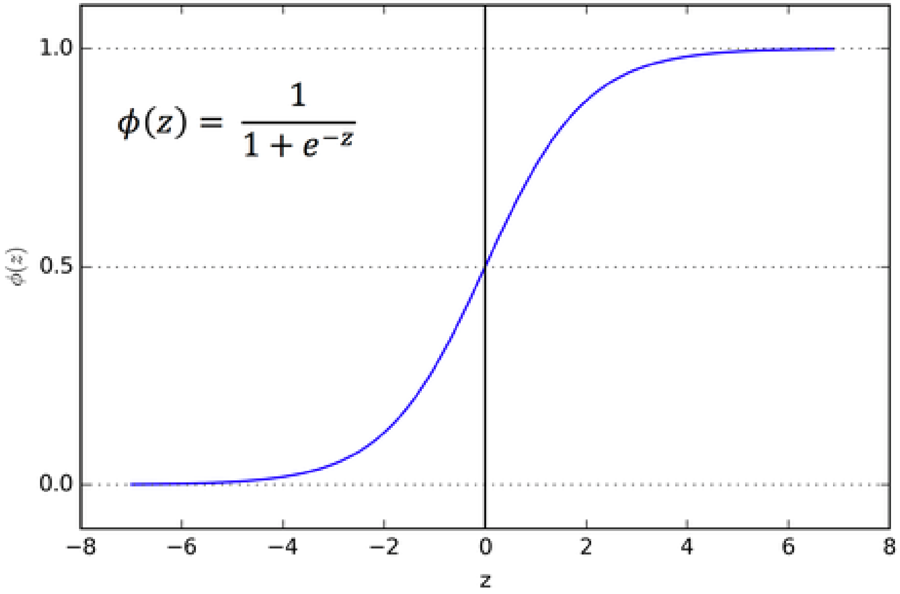


How to get probabilistic decisions?

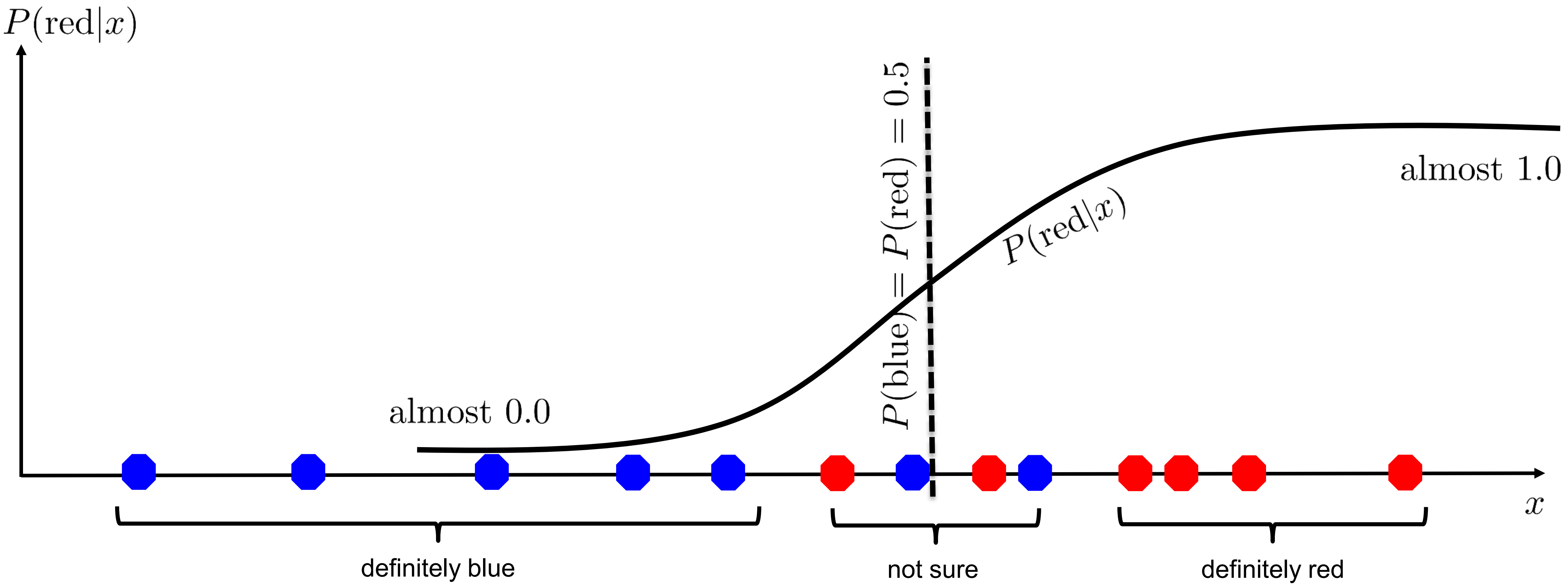
- Perceptron scoring: $z = w \cdot f(x)$
- If $z = w \cdot f(x)$ very positive → want probability going to 1
- If $z = w \cdot f(x)$ very negative → want probability going to 0

- Sigmoid function

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



A 1D Example

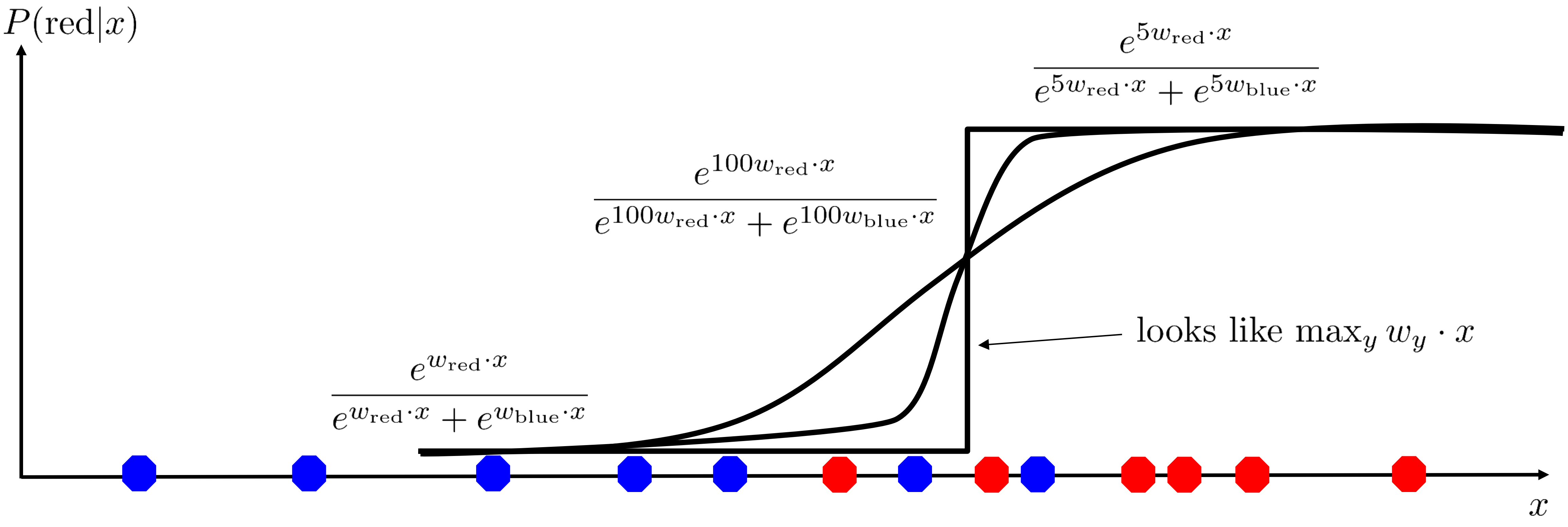


$$P(\text{red}|x) = \frac{e^{w_{\text{red}} \cdot x}}{e^{w_{\text{red}} \cdot x} + e^{w_{\text{blue}} \cdot x}}$$

probability increases exponentially as we move away from boundary (numerator)

normalizer (denominator)

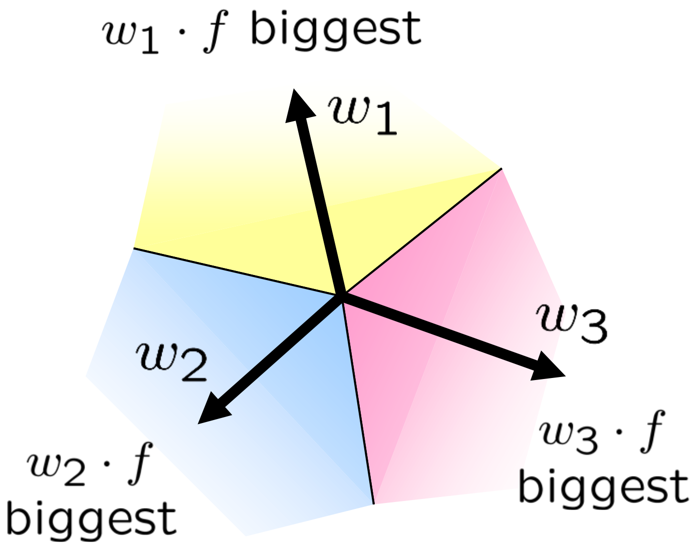
The *Soft* Max



$$P(\text{red}|x) = \frac{e^{w_{\text{red}}\cdot x}}{e^{w_{\text{red}}\cdot x}+e^{w_{\text{blue}}\cdot x}}$$

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 $y = \arg\max_y \; w_y \cdot f(x)$



- How to make the scores into probabilities?

$$\underbrace{z_1, z_2, z_3}_{\text{original activations}} \rightarrow \underbrace{\frac{e^{z_1}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_2}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}}}_{\text{softmax activations}}$$

Best w?

- Maximum likelihood estimation:

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

with:

$$P(y^{(i)}|x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_y e^{w_y \cdot f(x^{(i)})}}$$

= Multi-Class Logistic Regression

How do we learn in this setting?

- Optimization
  - i.e., how do we solve:

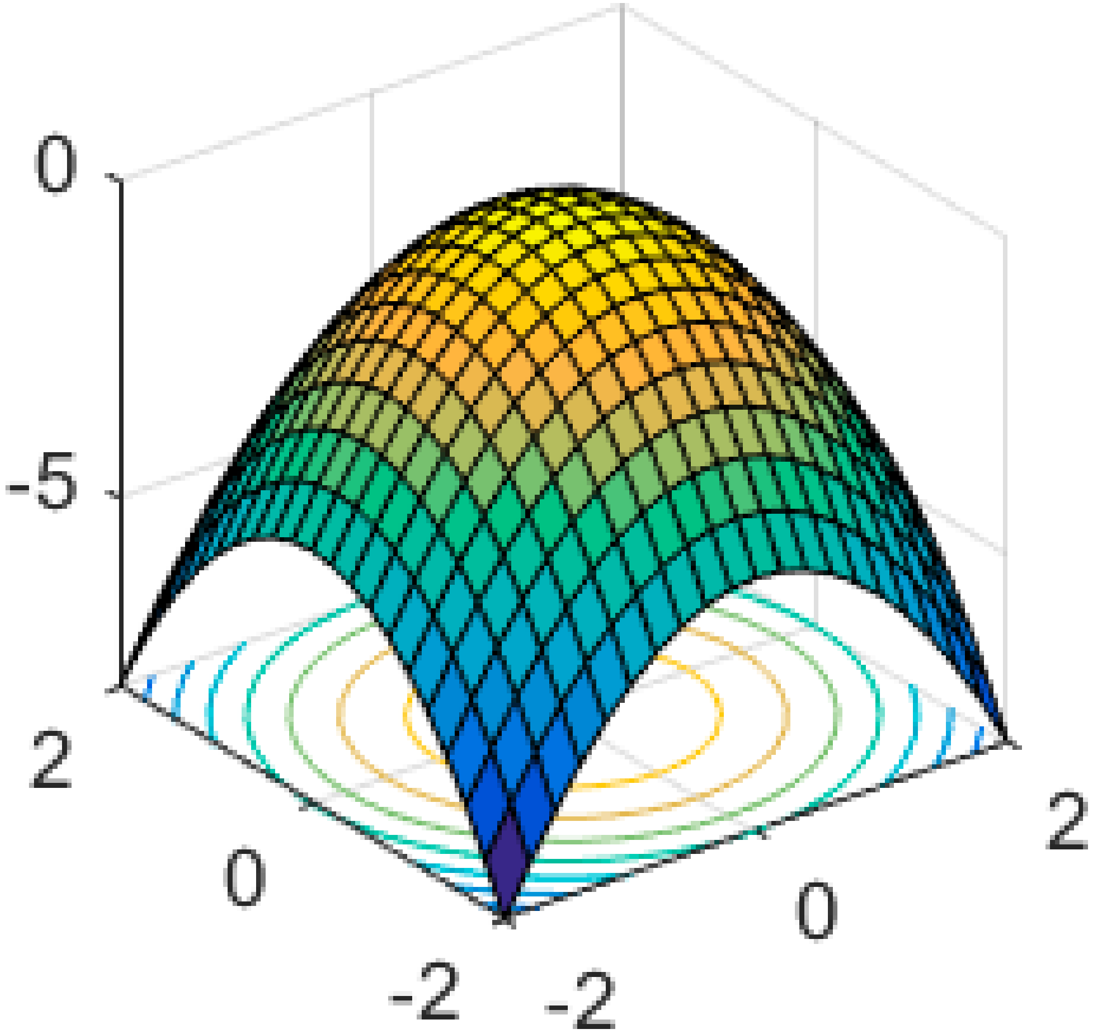
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)} | x^{(i)}; w)$$

Hill Climbing

- 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?

Optimization



Source: offconvex.org

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:

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

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

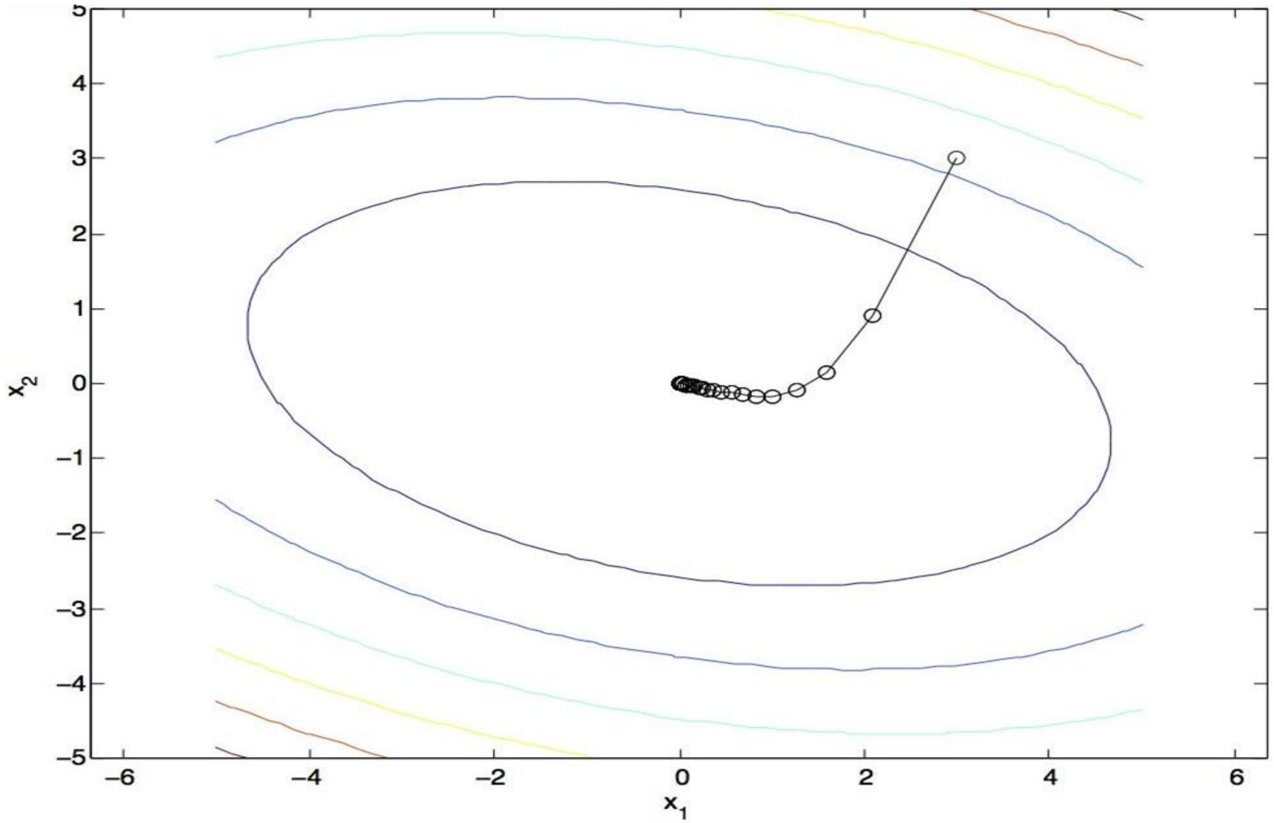


Figure source: Mathworks

Gradient in n dimensions

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

Optimization Procedure: Gradient Ascent

```
▪ Init w
▪ for iter = 1, 2, …
```

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

- α: learning rate --- tweaking parameter that needs to be chosen carefully
- How? Try multiple choices

Batch Gradient Ascent on the Log Likelihood Objective

$$\max_w \quad ll(w) = \max_w \quad \underbrace{\sum_i \log P(y^{(i)}|x^{(i)}; w)}_{g(w)}$$

- init w
- for iter = 1, 2, …

$$w \leftarrow w + \alpha * \sum_i \nabla \log P(y^{(i)}|x^{(i)}; w)$$

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

- init *w*
- for iter = 1, 2, …
  - pick random j

    $$w \leftarrow w + \alpha * \nabla \log P(y^{(j)}|x^{(j)}; w)$$

Mini-Batch Gradient Ascent on the Log Likelihood Objective

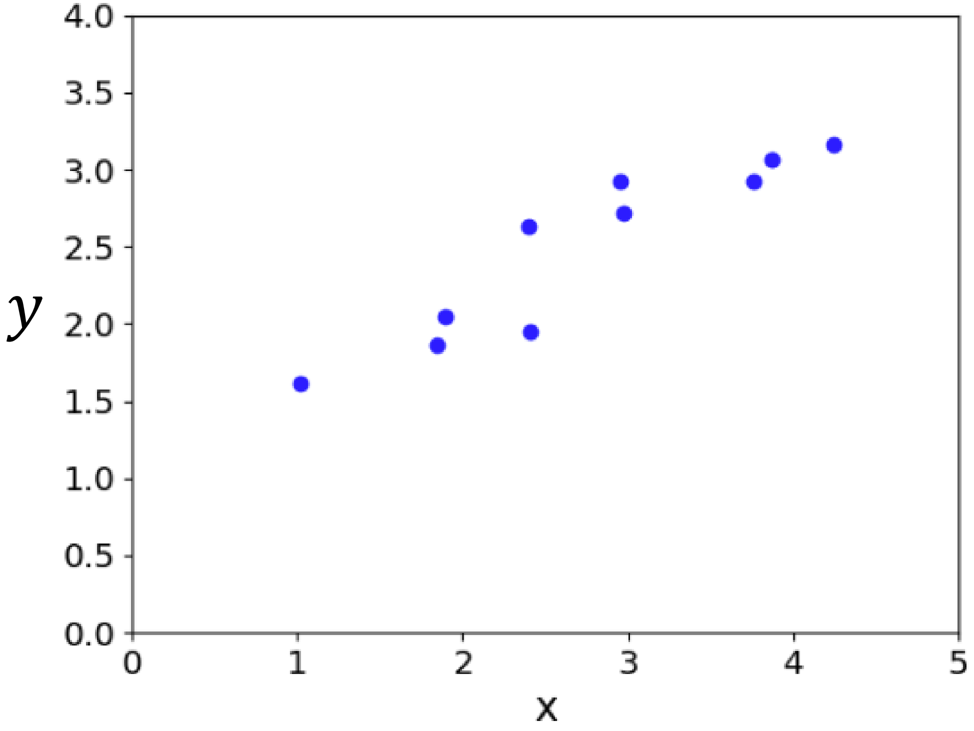
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

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

- `init` w
- `for iter = 1, 2, …`
  - `pick random subset of training examples J`

$$w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)}|x^{(j)}; w)$$

Regression



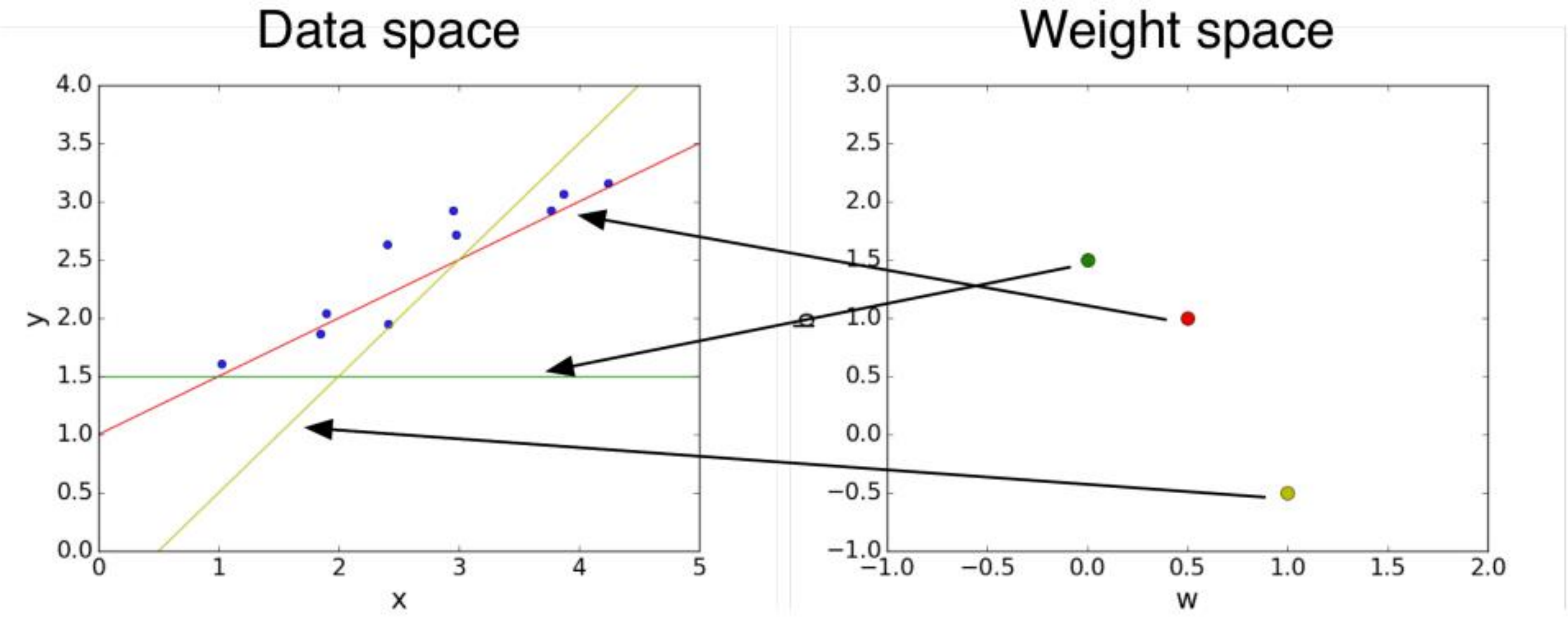
Linear Regression

- Learn to map from inputs x to outputs $y \in \mathbb{R}$
- $\hat{y} = w^T f(x) = w \circ f(x) = \sum_{i=1}^{d} w_i \cdot x_i$
  - Where $f(x)$ maps from the raw input x into a set of features

- How can we measure how good a set of weights w are?
  - Loss Function
    - Squared Error

$$\mathcal{L}(w) = \frac{1}{2}(y - \hat{y})^2 = \frac{1}{2}\left(y - w^T f(x)\right)^2$$

Linear Regression



- We want to find w that minimizes this loss function

$$\mathcal{L}(w) = \frac{1}{2}(y - \hat{y})^2 = \frac{1}{2}\left(y - w^T f(x)\right)^2$$

- Calculus to the rescue!

$$\frac{\partial \mathcal{L}}{\partial w_i} = -\left(y - w^T f(x)\right) f_i(x) = (w^T f(x) - y) f_i(x)$$

Linear Regression

- How can we measure how good a set of weights w are?
  - Mean Squared Error

$$\mathcal{L}_{MSE}(w) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}(y_i - \hat{y}_i)^2 = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}\left(y_i - w^T f(x)\right)^2$$

$$\frac{\partial \mathcal{L}_{MSE}}{\partial w_i} = \frac{1}{N}\sum_{i=1}^{N}(w^T f(x) - y) f_i(x)$$

How to optimize?

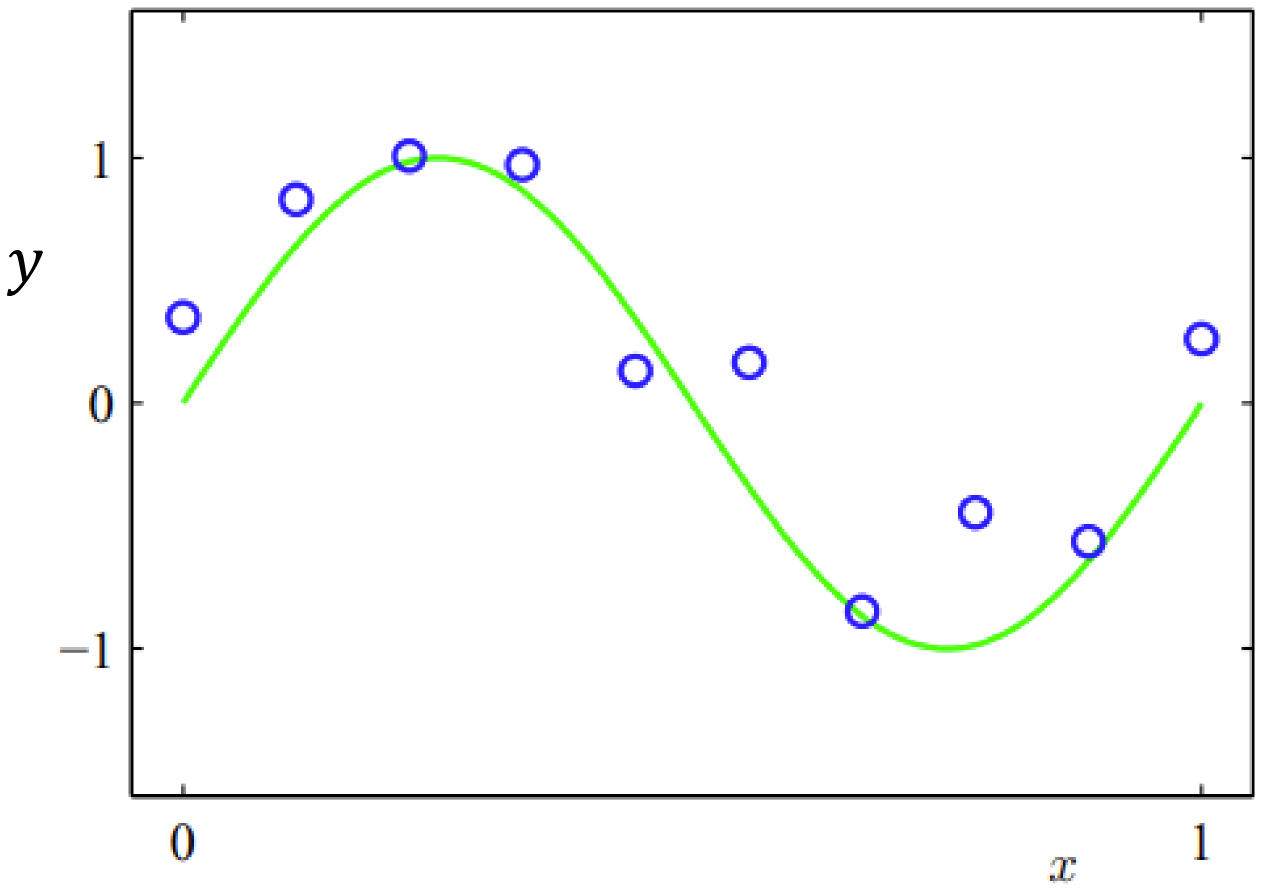
- Gradient Descent

```
▪ Init w
▪ for iter = 1, 2, …
```

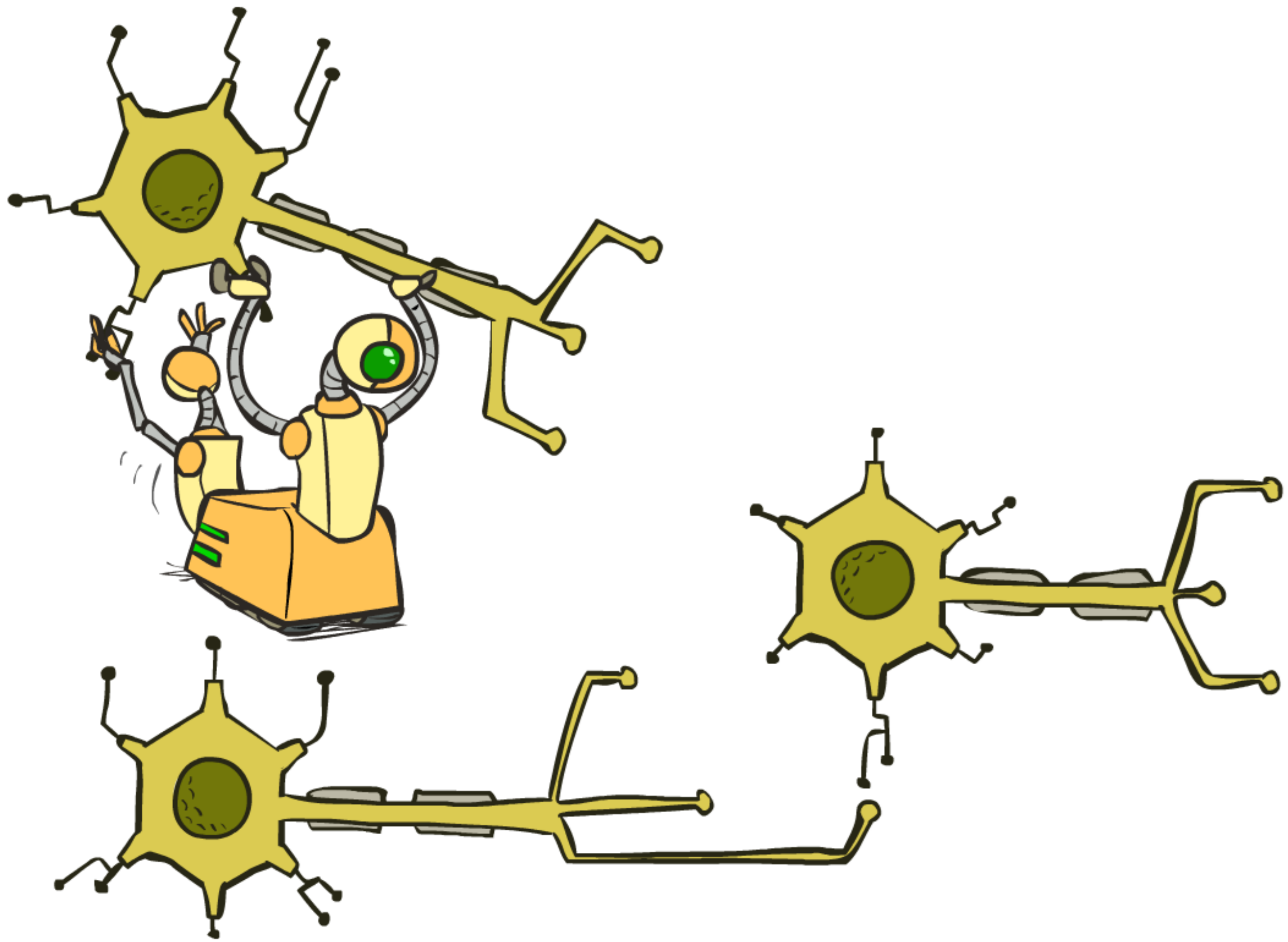
$$w \leftarrow w - \alpha \cdot \nabla \mathcal{L}(w)$$

- Usually we will use stochastic gradient descent using mini-batches, just like we talked about for classification.

Non-Linear Regression?

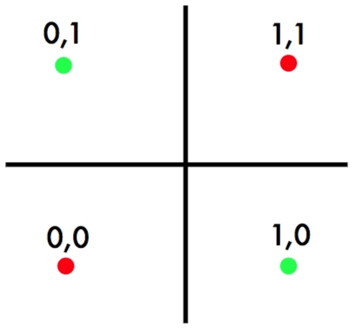


Neural Networks



History Lesson

- 1943: Artificial Neuron
  - McCulloch and Pitts showed simple threshold logic
- 1957: Perceptron
  - Rosenblatt introduced algorithm for single-layer neural network
  - Explored “Multi-Layer Perceptrons” but lacked good learning algorithms
- 1969: AI Winter
  - Minsky and Papert publish book called “Perceptrons”

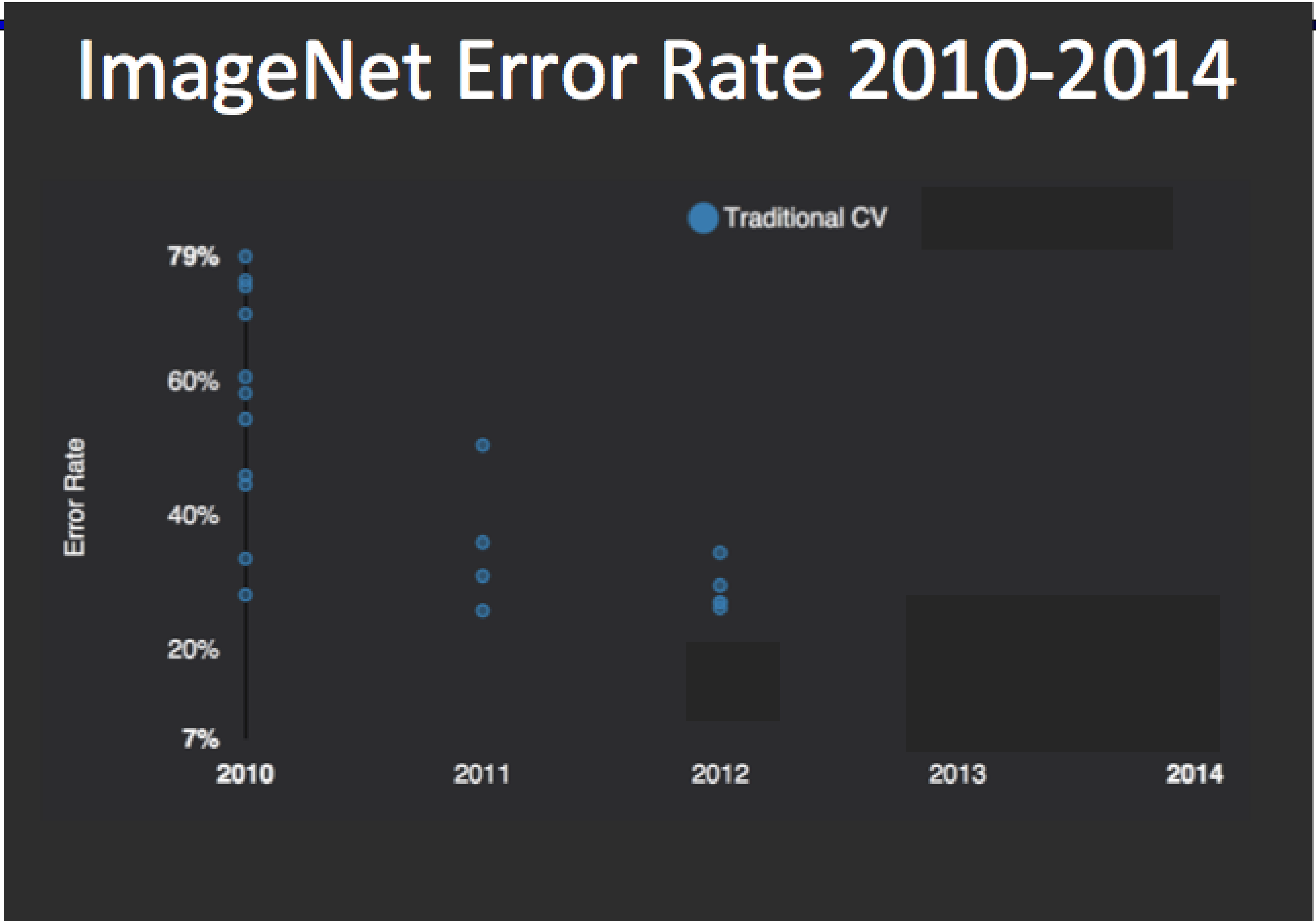


XOR

History Lesson

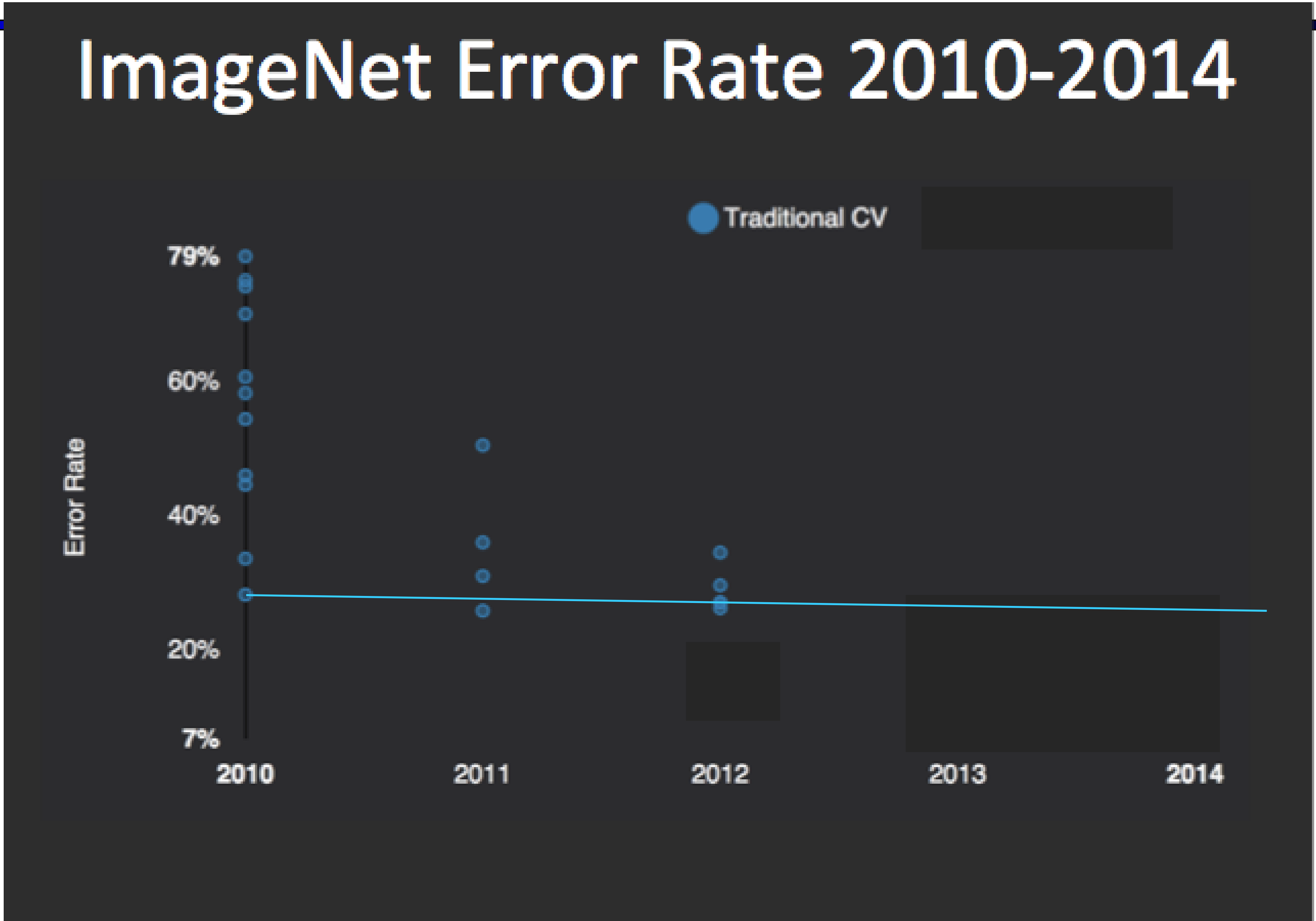
- 1986: Backpropagation
  - Rumelhart, Hinton, and Williams show power of multi-layer perceptrons trained via backpropagation
- Early 2010s: Hardware and algorithms converge with big data
- 2012: AlexNet and the image recognition breakthrough
- 2012–present: The deep learning era

Performance



graph credit Matt Zeiler, Clarifai

Performance



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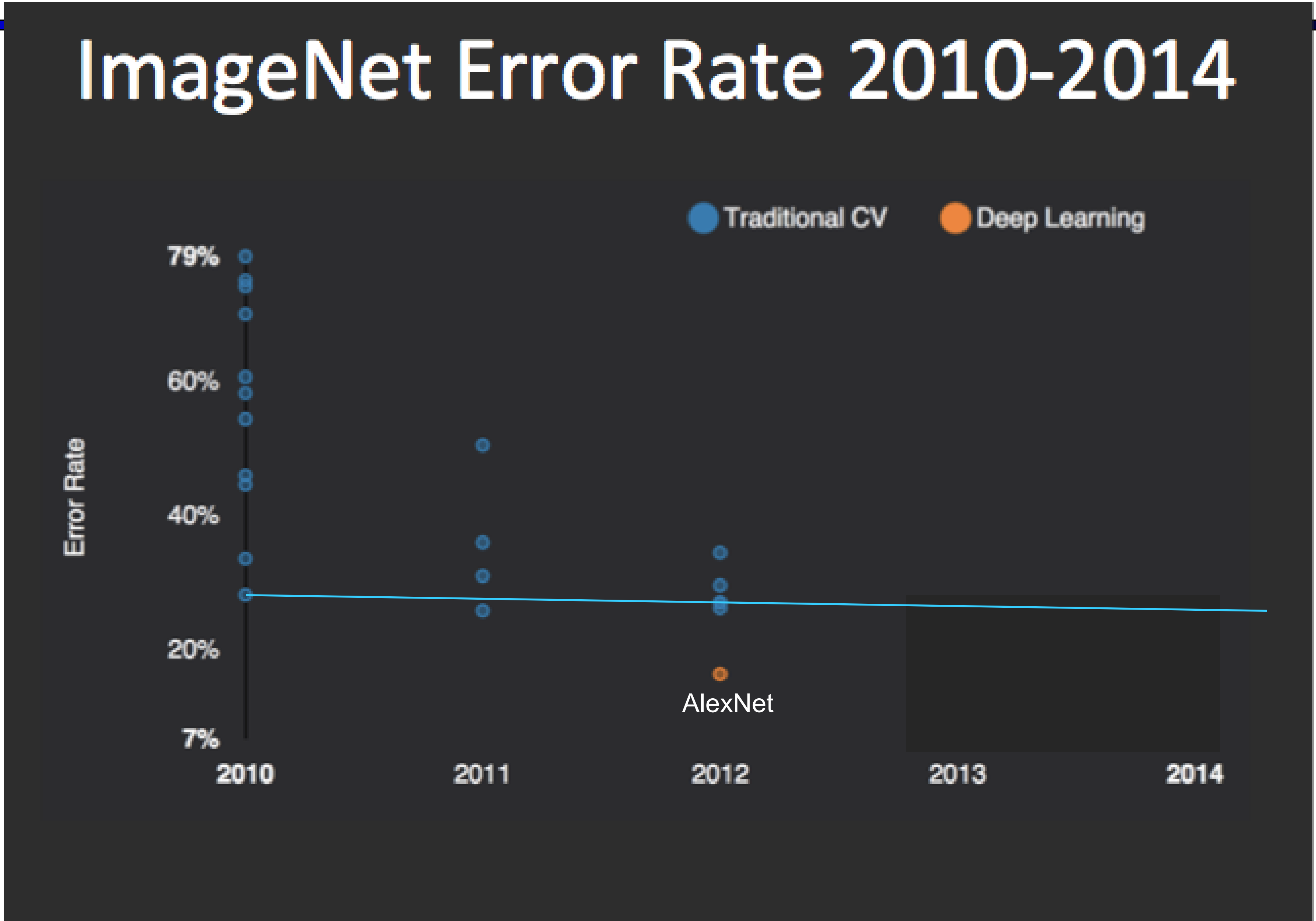
Performance



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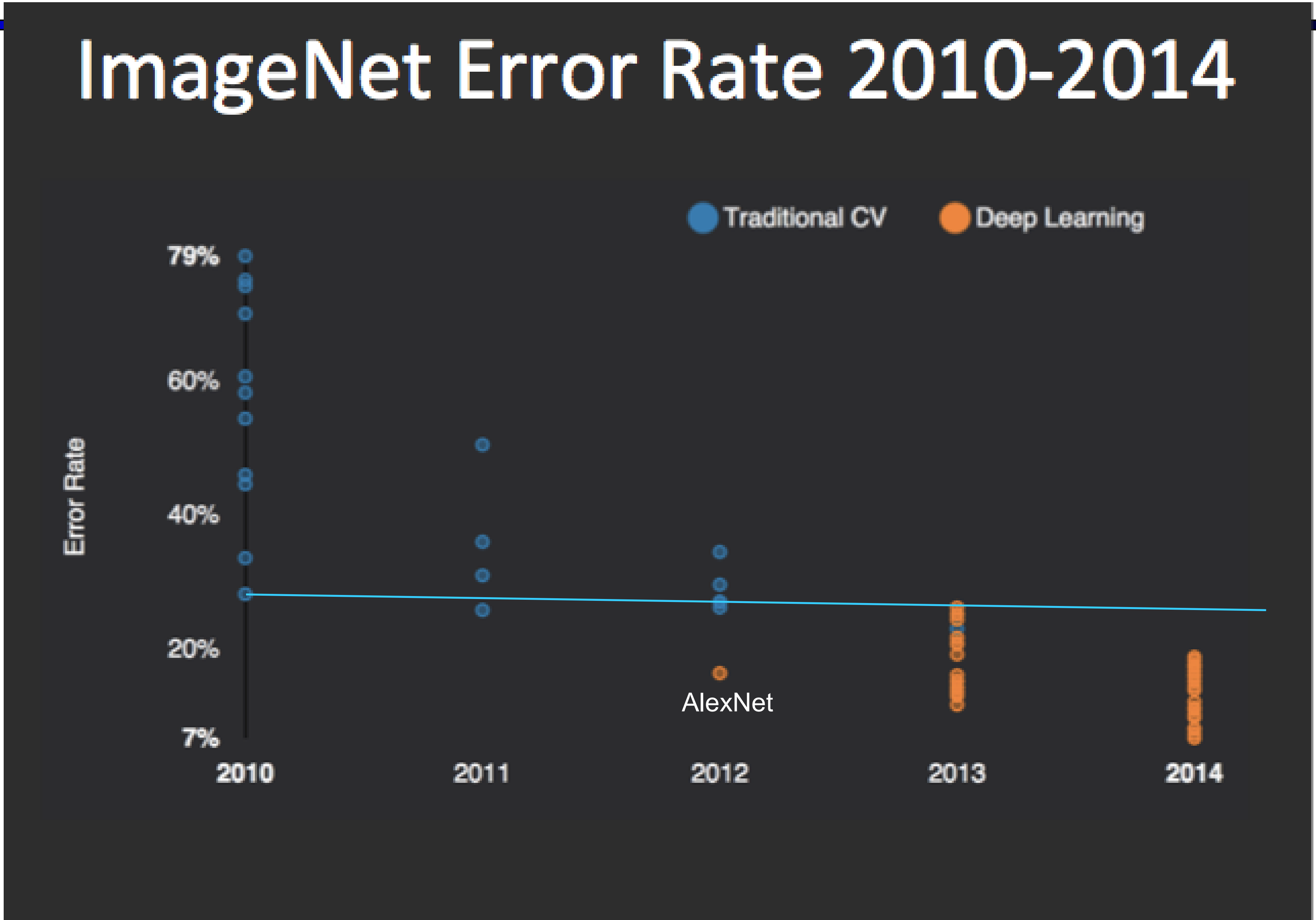
Performance



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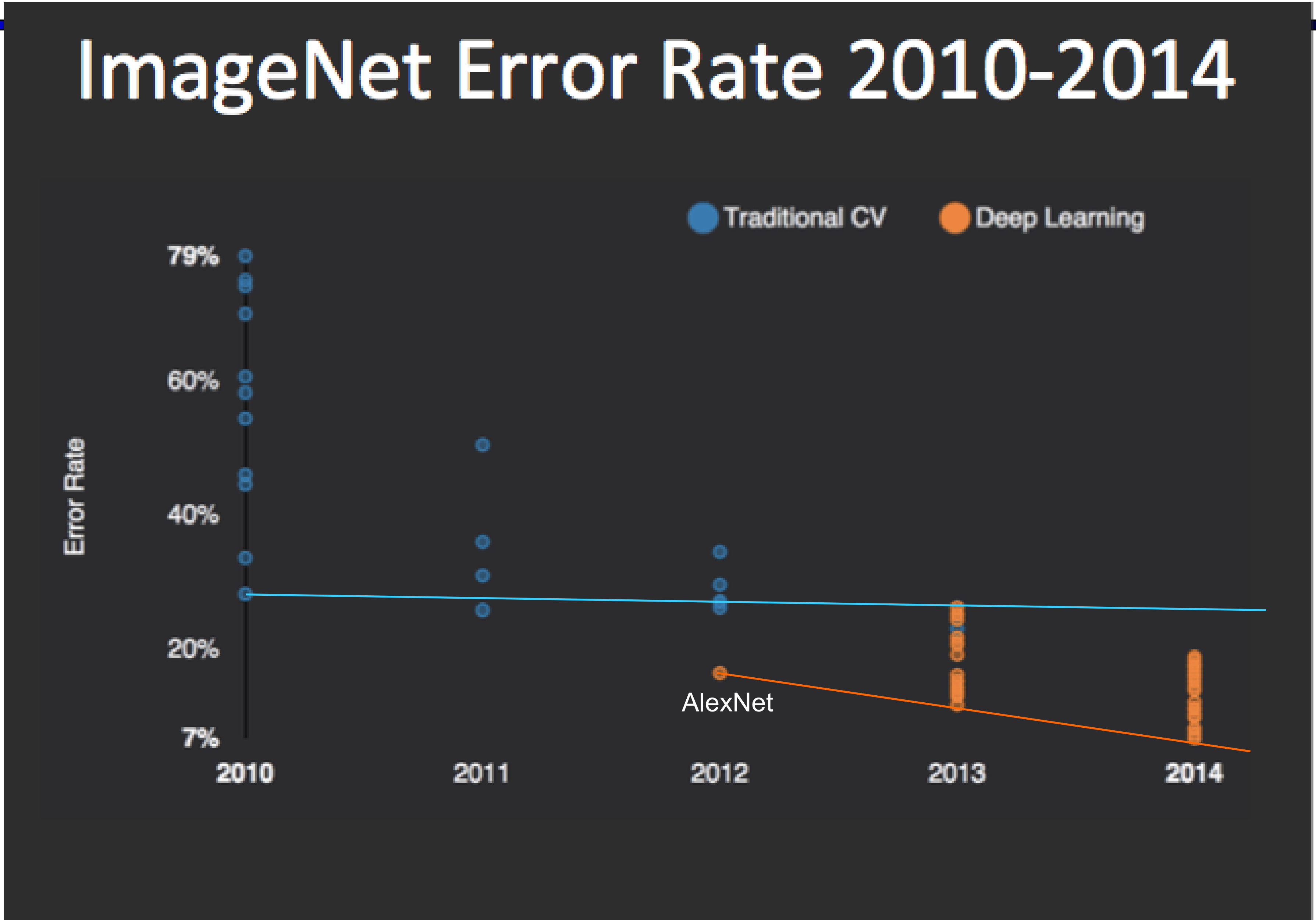
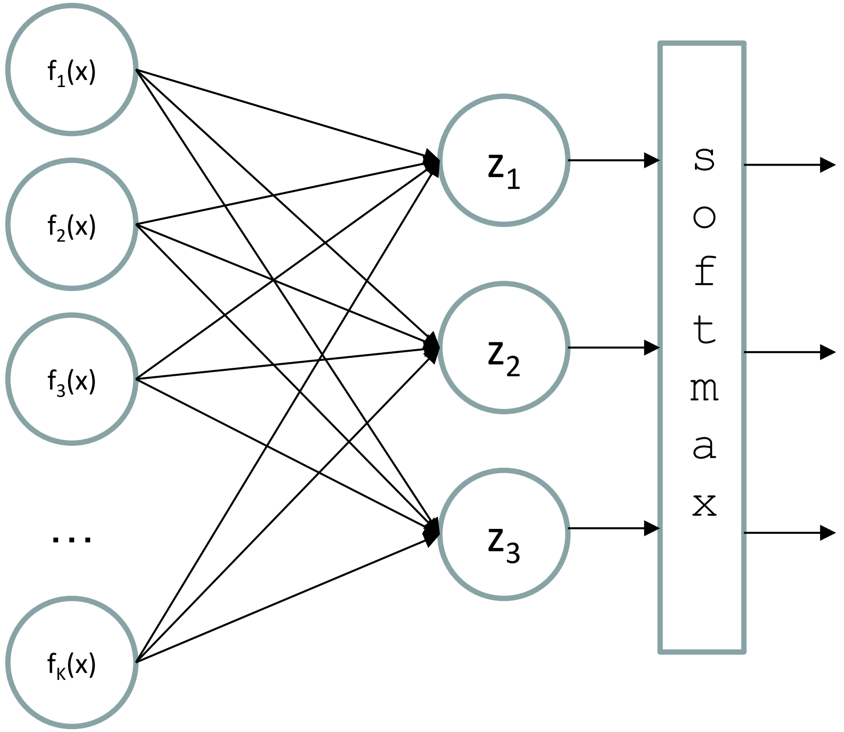
Performance



graph credit Matt Zeiler, Clarifai

Multi-class Logistic Regression

- = special case of neural network

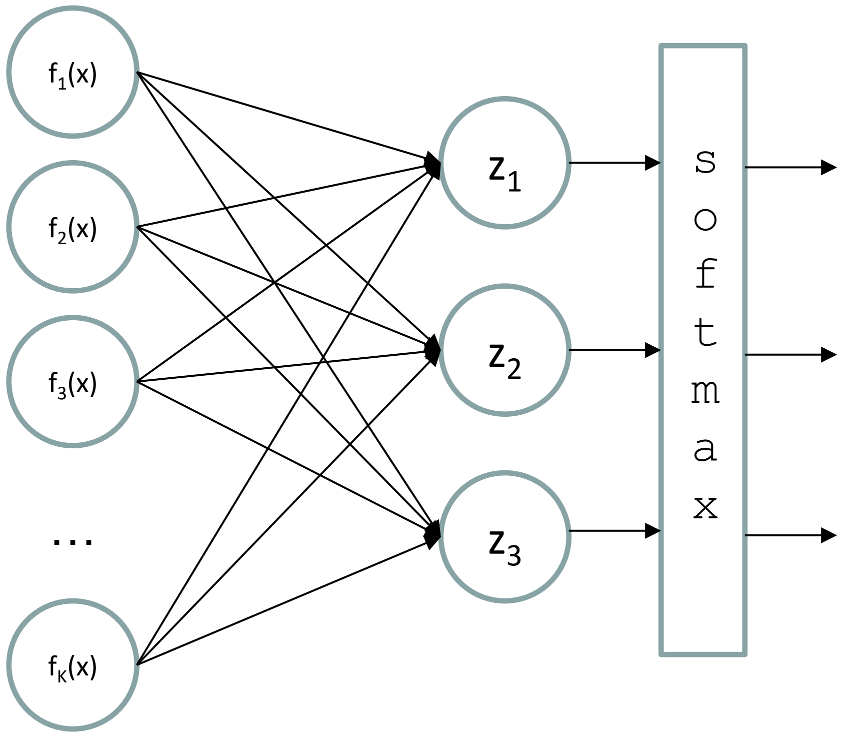


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_2|x;w) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

Deep Neural Network = Also learn the features!

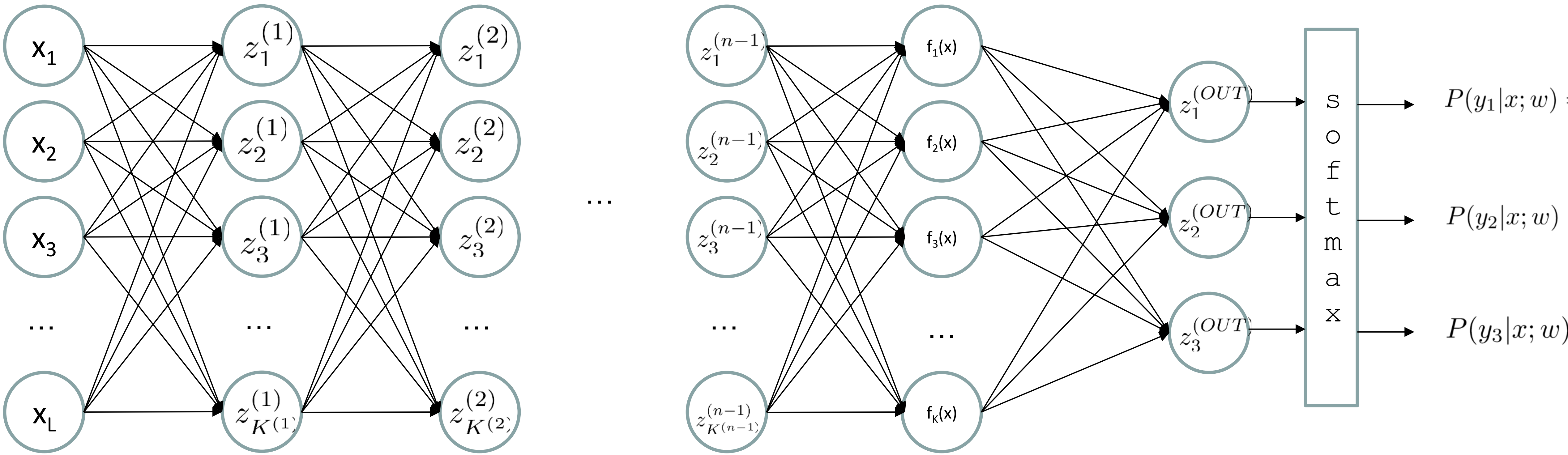


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_2|x;w) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

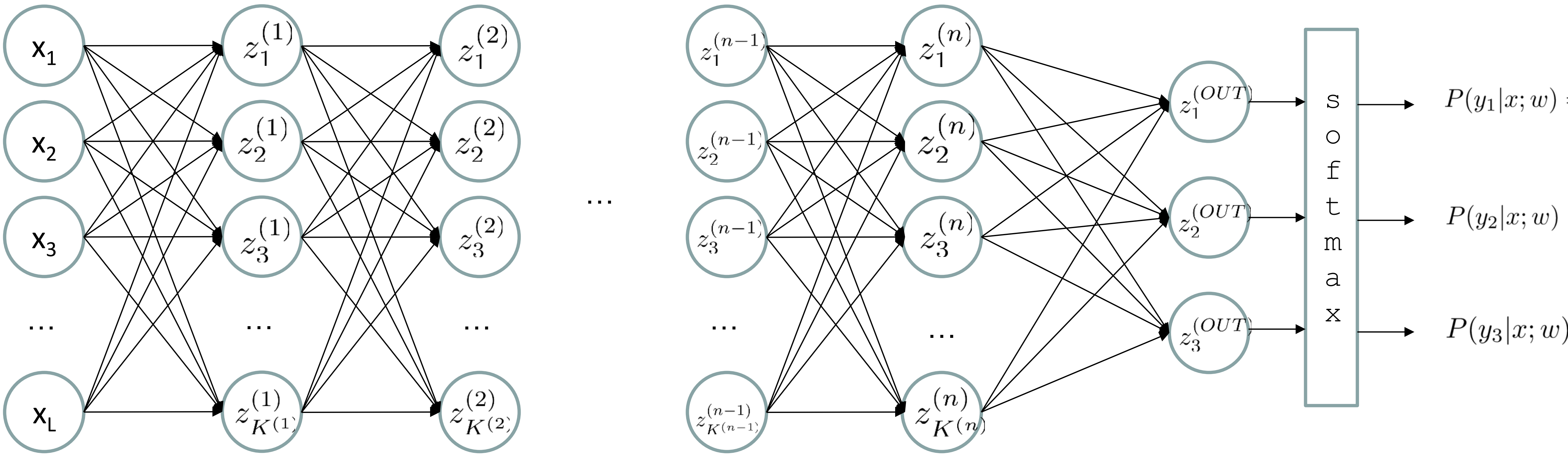
Deep Neural Network = Also learn the features!



$$z_i^{(k)} = g(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

g = nonlinear activation function

Deep Neural Network = Also learn the features!

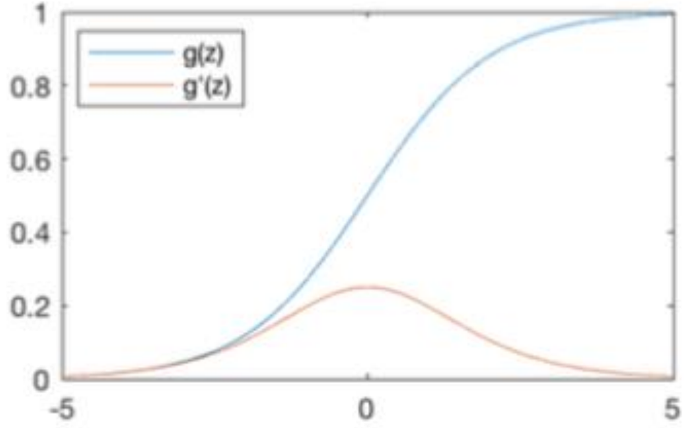


$$z_i^{(k)} = g\left(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)}\right)$$

g = nonlinear activation function

Common Activation Functions

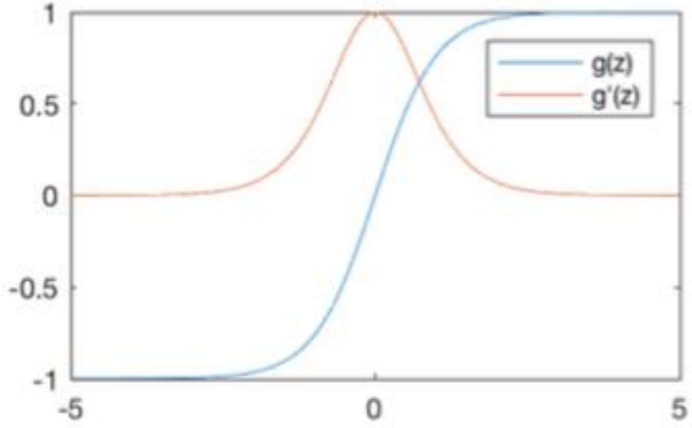
Sigmoid Function



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

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

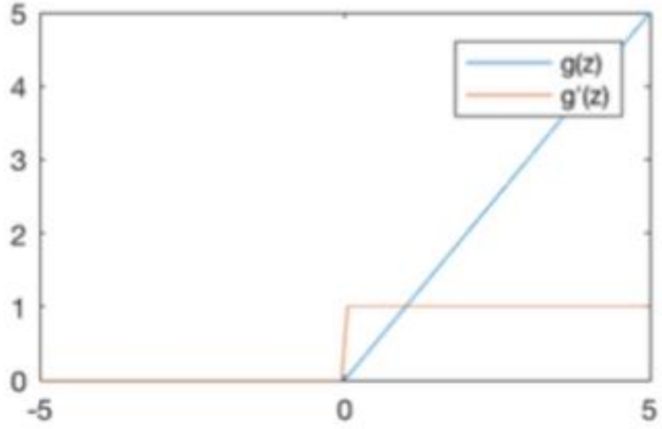
Hyperbolic Tangent



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

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



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

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

Deep Neural Network: Also Learn the Features!

- Training the deep neural network is just like logistic regression:

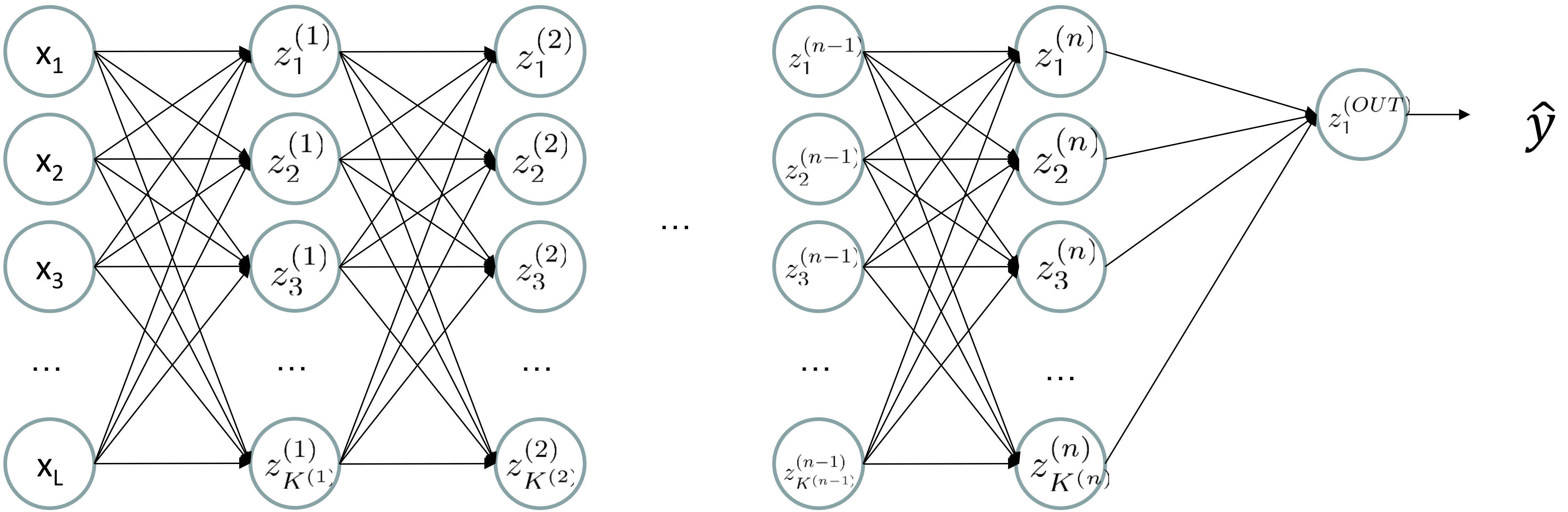
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

just w tends to be a much, much larger vector ☺

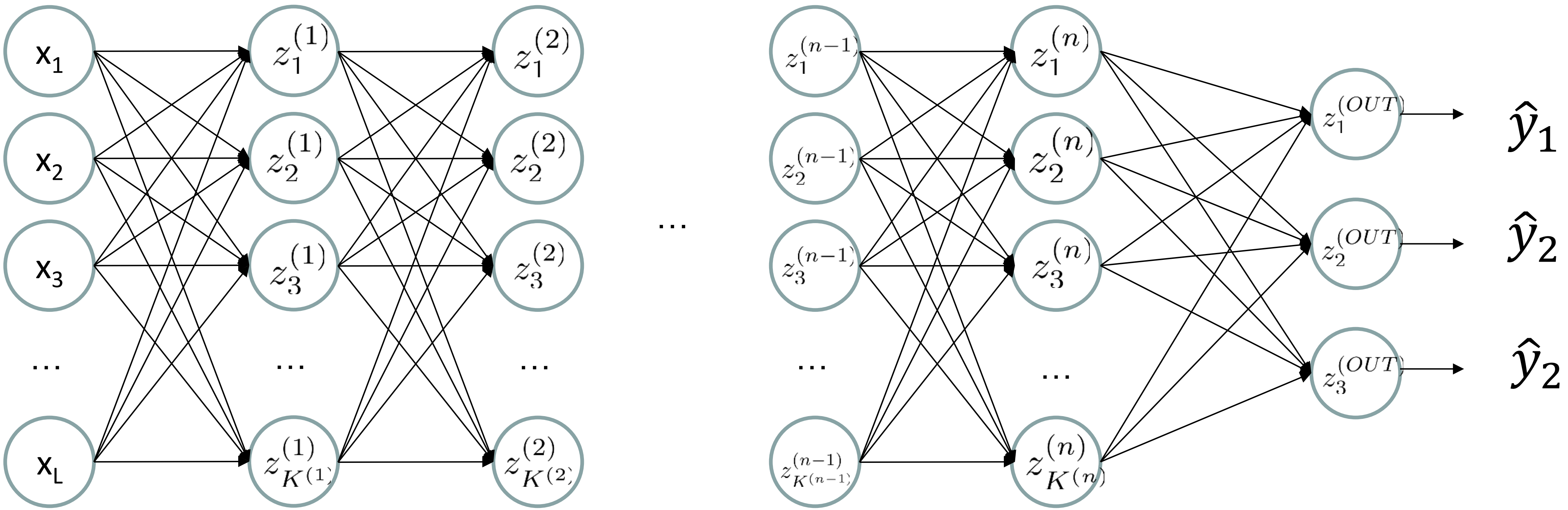
- just run gradient ascent

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

Deep Neural Networks for Regression



Deep Neural Networks for Regression



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.

Fun Neural Net Demo Site

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

How about computing all the derivatives?

- Derivatives tables:

$$\frac{d}{dx}(a) = 0$$

$$\frac{d}{dx}(x) = 1$$

$$\frac{d}{dx}(au) = a\frac{du}{dx}$$

$$\frac{d}{dx}(u + v - w) = \frac{du}{dx} + \frac{dv}{dx} - \frac{dw}{dx}$$

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{u}{v}\right) = \frac{1}{v}\frac{du}{dx} - \frac{u}{v^2}\frac{dv}{dx}$$

$$\frac{d}{dx}(u^n) = nu^{n-1}\frac{du}{dx}$$

$$\frac{d}{dx}(\sqrt{u}) = \frac{1}{2\sqrt{u}}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u}\right) = -\frac{1}{u^2}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u^n}\right) = -\frac{n}{u^{n+1}}\frac{du}{dx}$$

$$\frac{d}{dx}[f(u)] = \frac{d}{du}[f(u)]\frac{du}{dx}$$

$$\frac{d}{dx}[\ln u] = \frac{d}{dx}[\log_e u] = \frac{1}{u}\frac{du}{dx}$$

$$\frac{d}{dx}[\log_a u] = \log_a e\frac{1}{u}\frac{du}{dx}$$

$$\frac{d}{dx}e^u = e^u\frac{du}{dx}$$

$$\frac{d}{dx}a^u = a^u \ln a\frac{du}{dx}$$

$$\frac{d}{dx}\left(u^v\right) = vu^{v-1}\frac{du}{dx} + \ln u \quad u^v\frac{dv}{dx}$$

$$\frac{d}{dx}\sin u = \cos u\frac{du}{dx}$$

$$\frac{d}{dx}\cos u = -\sin u\frac{du}{dx}$$

$$\frac{d}{dx}\tan u = \sec^2 u\frac{du}{dx}$$

$$\frac{d}{dx}\cot u = -\csc^2 u\frac{du}{dx}$$

$$\frac{d}{dx}\sec u = \sec u \tan u\frac{du}{dx}$$

$$\frac{d}{dx}\csc u = -\csc u \cot u\frac{du}{dx}$$

[source: http://hyperphysics.phy-astr.gsu.edu/hbase/Math/derfunc.html

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

Derivatives can be computed by following well-defined procedures

Automatic Differentiation

- Automatic differentiation software
  - e.g. PyTorch, TensorFlow, 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? -- outside of scope of our class