Supervised Machine Learning

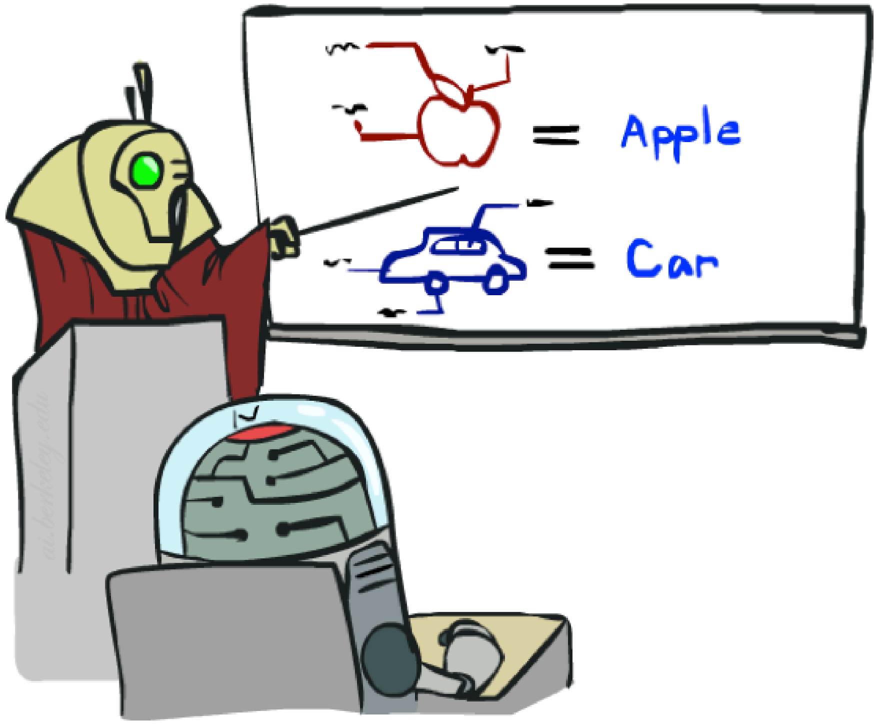
AIMA Chapter 18, 20

[Adapted from slides by Dan Klein and Pieter Abbeel at UC Berkeley]

Supervised learning

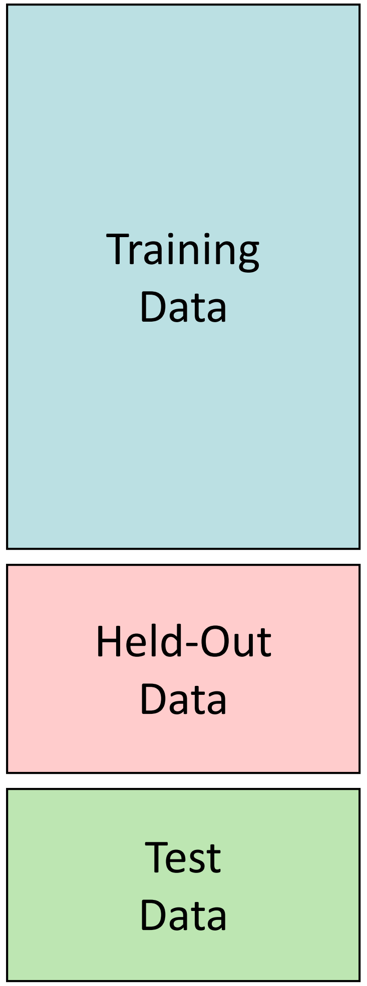
- To learn an unknown *target function* f
- Input: a *training set* of *labeled examples* (x_j, y_j) where $y_j = f(x_j)$
- Output: *hypothesis* h that is "close" to f

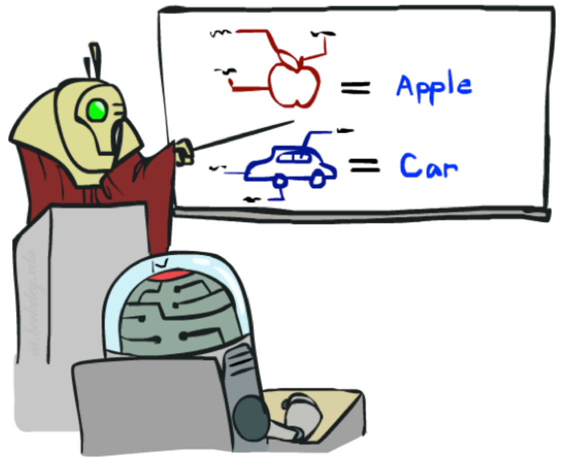
- Types of supervised learning
  - Classification = learning f with discrete output value
  - Regression = learning f with real-valued output value
  - Structured prediction = learning f with structured output



Important Concepts

- Data: labeled instances, e.g. emails marked spam/ham
  - Training set
  - Held out set
  - Test set
- Experimentation cycle
  - Learn parameters (e.g. model probabilities) on training set
  - Tune hyperparameters on held-out set
  - Compute accuracy of test set (fraction of instances predicted correctly)
  - Very important: never “peek” at the test set!





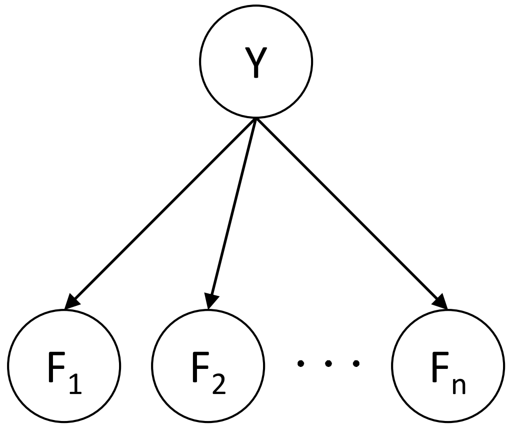
Naïve Bayes

- Naive Bayes model:

|Y| parameters

$$P(\mathsf{Y}, \mathsf{F}_1 \dots \mathsf{F}_n) = \quad P(\mathsf{Y}) \prod_i P(\mathsf{F}_i | \mathsf{Y})$$

n x |F| x |Y| parameters



- Assume all features are independent effects of the label

- Total number of parameters is *linear* in n
- Tree-structured: *linear* inference time
- Model is very simplistic, but often works anyway

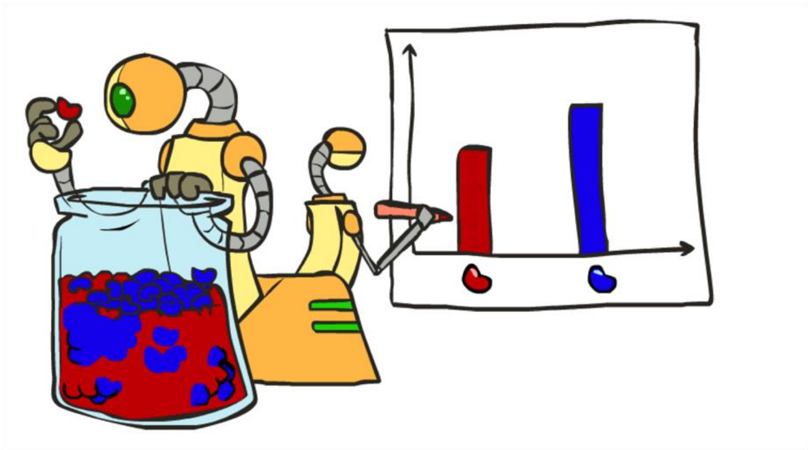
Parameter Estimation

- Estimating the distribution of a random variable
- *Elicitation:* ask a human (this is hard…)
- *Empirically:* use training data (learning!)
  - For each outcome x, look at the *empirical rate* of that value

$$P_{\text{ML}}(x) = \frac{\text{count}(x)}{\text{total samples}}$$

  - Ex:
    - We've seen 1000 words from spam emails, among which we see "money" for 50 times
    - So we set P(money | spam) = 0.05

  - This is the estimate that maximizes the *likelihood of the data*
    - Likelihood: conditional probability of the data given the parameters



Generalization and Overfitting

- Overfitting: learn to fit the training data very closely, but fit the test data poorly
  - Generalization: try to fit the test data as well
- Why does overfitting occur?
  - Training data is not representative of the true data distribution
    - Too few training samples
    - Training data is noisy
  - Too many attributes, some of them irrelevant to the classification task
  - The model is too expressive
    - Ex: the model is capable of memorizing all the spam emails in the training set

Generalization and Overfitting

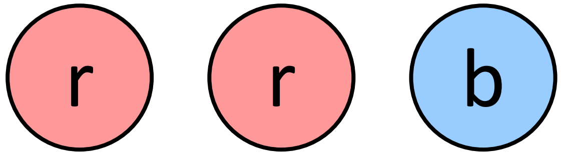
- Avoid overfitting
  - Acquire more training data (not always possible)
  - Remove irrelevant attributes (not always possible)
  - Limit the model expressiveness by regularization, early stopping, pruning, etc.
- In our previous example, we may smooth the empirical rate to improve generalization

Laplace Smoothing

- Laplace's estimate:
  - Pretend you saw every outcome once more than you actually did

$$P_{LAP}(x) = \frac{c(x)+1}{\sum_x [c(x)+1]}$$

$$= \frac{c(x)+1}{N+|X|}$$



$$P_{ML}(X) =$$

$$P_{LAP}(X) =$$

  - Can derive this estimate with *Dirichlet priors* (see cs281a)

Laplace Smoothing

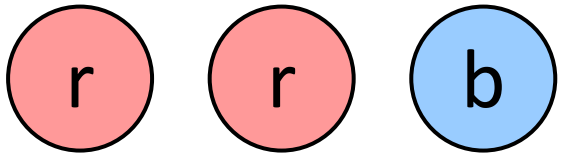
- Laplace's estimate (extended):
  - Pretend you saw every outcome k extra times

$$P_{LAP,k}(x) = \frac{c(x) + k}{N + k|X|}$$

  - What's Laplace with k = 0?
  - k is the strength of the prior

- Laplace for conditionals:
  - Smooth each condition independently:

$$P_{LAP,k}(x|y) = \frac{c(x,y) + k}{c(y) + k|X|}$$



$$P_{LAP,0}(X) =$$

$$P_{LAP,1}(X) =$$

$$P_{LAP,100}(X) =$$

Real NB: Smoothing

- For real classification problems, smoothing is critical
- New odds ratios:

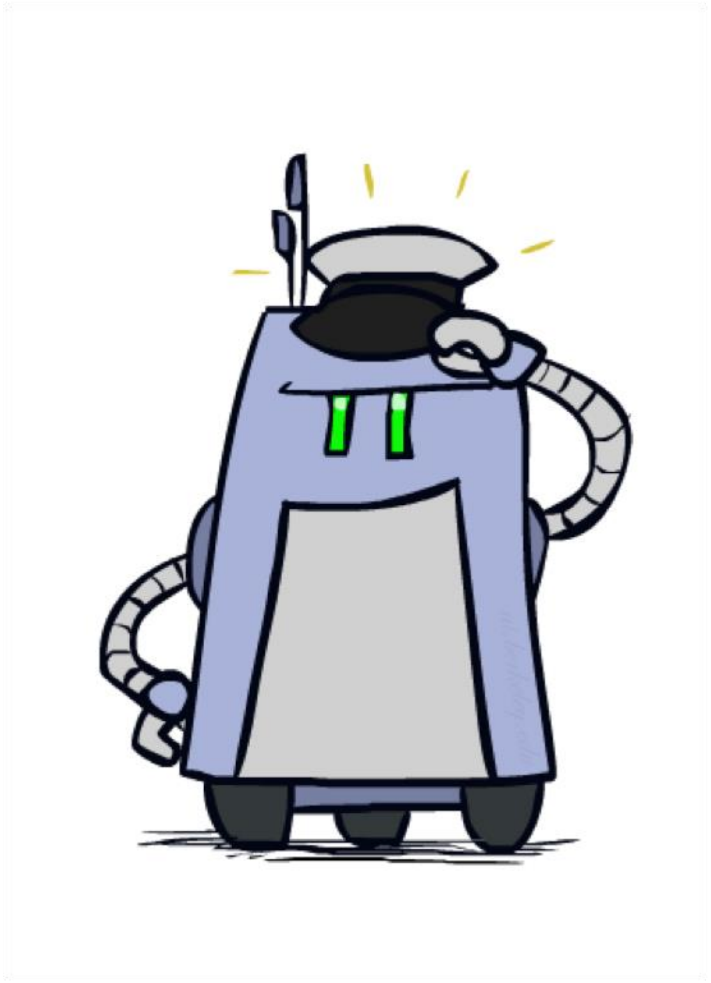
$$\frac{P(W|\text{ham})}{P(W|\text{spam})}$$

helvetica	:	11.4
seems	:	10.8
group	:	10.2
ago	:	8.4
areas	:	8.3
...		

$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

verdana	:	28.8
Credit	:	28.4
ORDER	:	27.2
<FONT>	:	26.9
money	:	26.5
...		

Do these make more sense?



Linear Interpolation

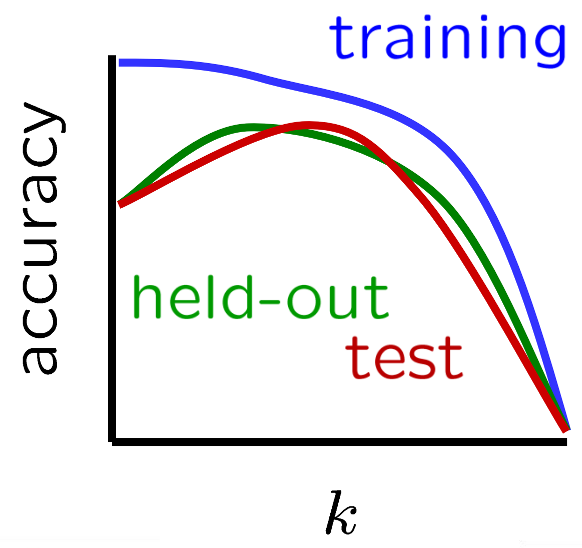
- In practice, Laplace often performs poorly for P(X|Y):
  - When |X| is very large
  - When |Y| is very large

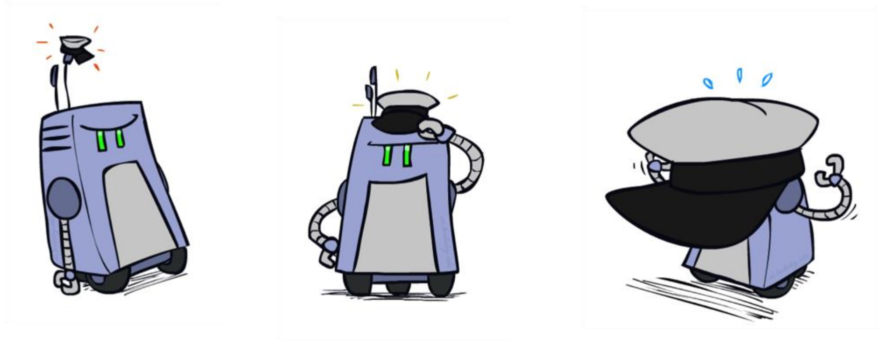
- Another option: linear interpolation
  - Also get the empirical P(X) from the data
  - Make sure the estimate of P(X|Y) isn't too different from the empirical P(X)

$$P_{LIN}(x|y) = \alpha \widehat{P}(x|y) + (1.0 - \alpha)\widehat{P}(x)$$

Tuning on Held-Out Data

- Now we've got two kinds of unknowns
  - Parameters: the probabilities P(X|Y), P(Y)
  - Hyperparameters: e.g. the amount / type of smoothing to do, k, α
- What should we learn where?
  - Learn parameters from training data
  - Tune hyperparameters on different data
    - Why?
  - For each value of the hyperparameters, train and test on the held-out data
  - Choose the best value and do a final test on the test data





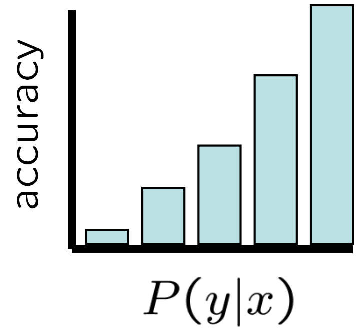
Confidences from a Classifier

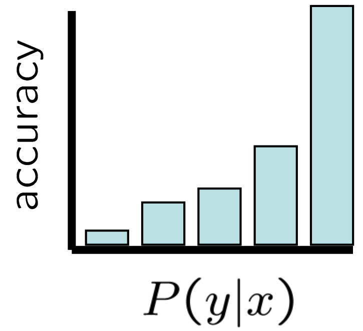
- The confidence of a probabilistic classifier:
  - Posterior over the top label

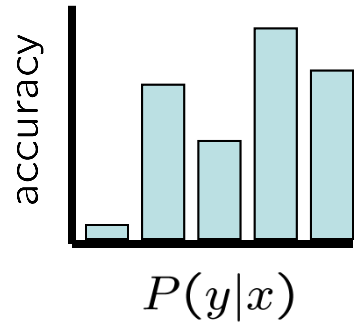
$$\text{confidence}(x) = \max_y P(y|x)$$

  - Represents how sure the classifier is of the classification
  - Any probabilistic model will have confidences
  - No guarantee confidence is correct

- Calibration
  - Weak calibration: higher confidences mean higher accuracy
  - Strong calibration: confidence predicts accuracy rate
  - What's the value of calibration?



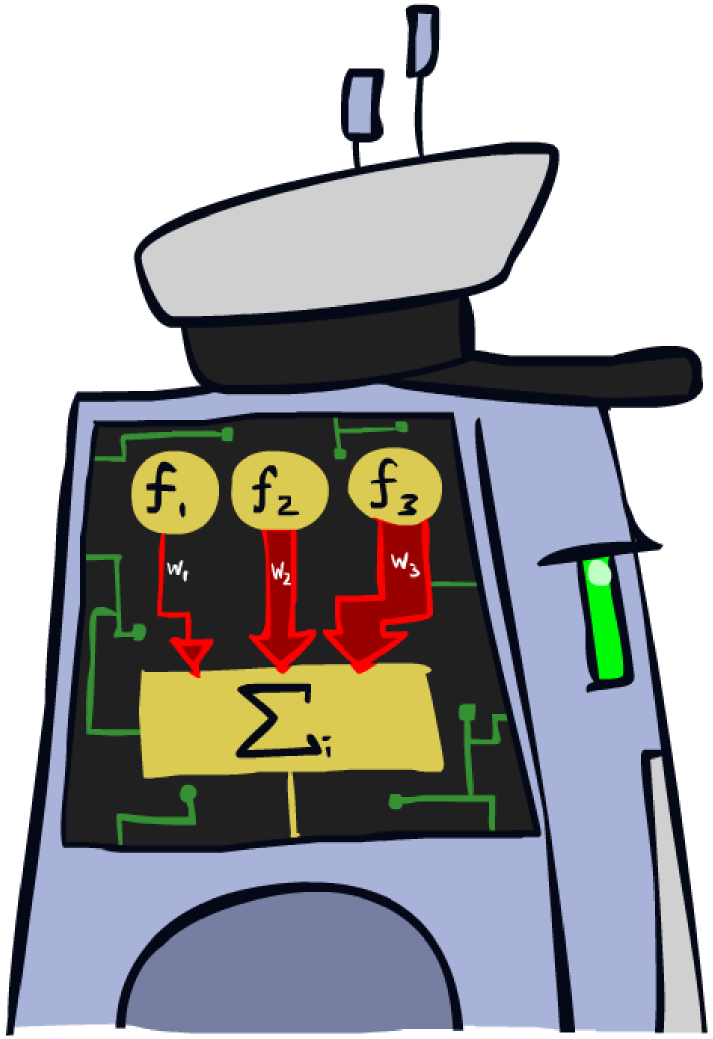




Summary

- Bayes rule lets us do diagnostic queries with causal probabilities
- The naïve Bayes assumption takes all features to be independent given the class label
- We can build classifiers out of a naïve Bayes model using training data
- Smoothing estimates is important in real systems
- Classifier confidences are useful, when you can get them

Linear Classifiers



Feature Vectors

x $\longrightarrow$ $f(x)$ $\longrightarrow$ y

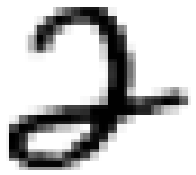
```
Hello,

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

$\Rightarrow$

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

$\Rightarrow$

SPAM
or
+



$\Rightarrow$

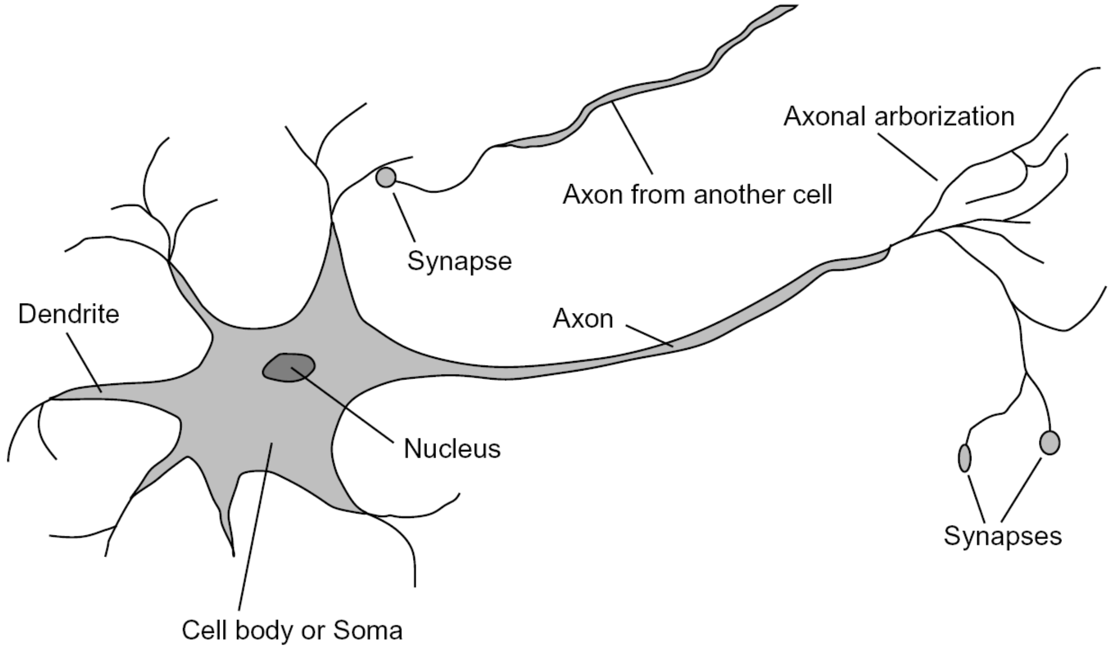
```
PIXEL-7,12   : 1
PIXEL-7,13   : 0
...
NUM_LOOPS    : 1
...
```

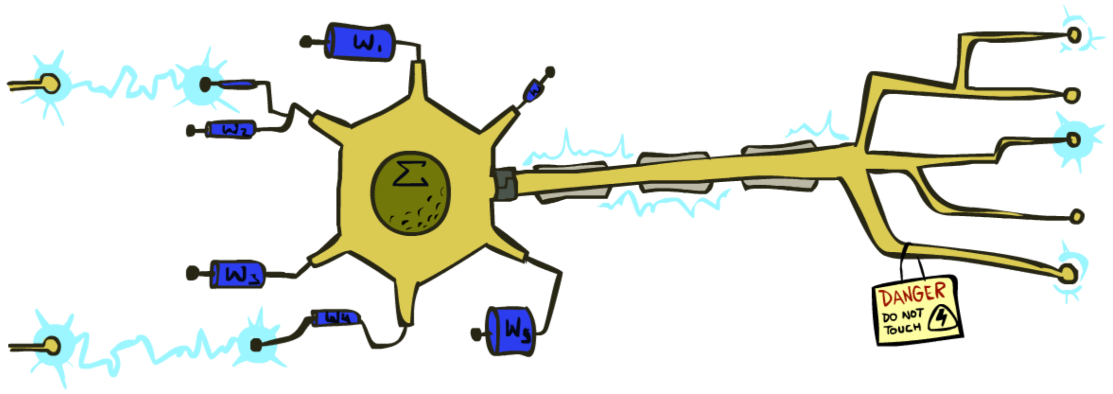
$\Rightarrow$

“2”

Some (Simplified) Biology

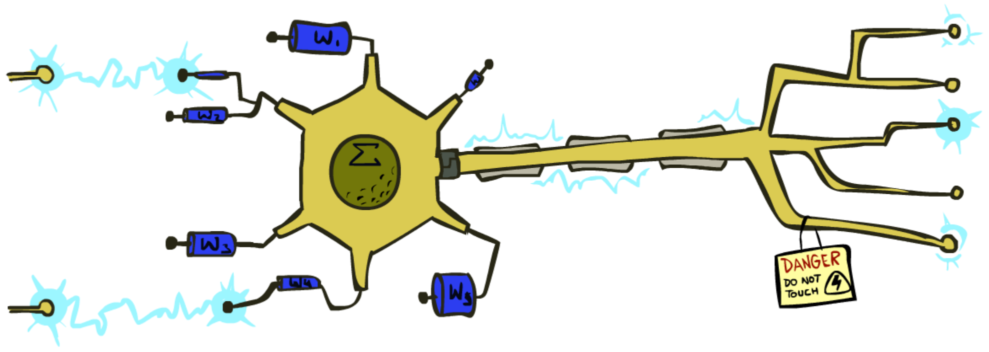
- Very loose inspiration: human neurons





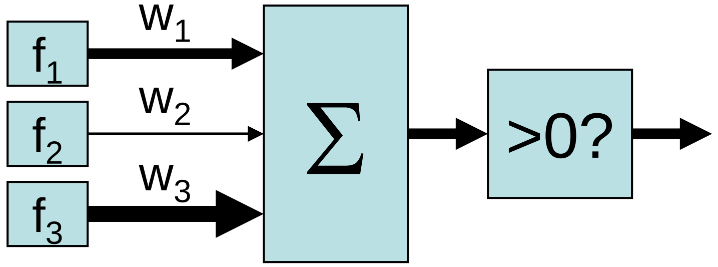
Linear Classifiers

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



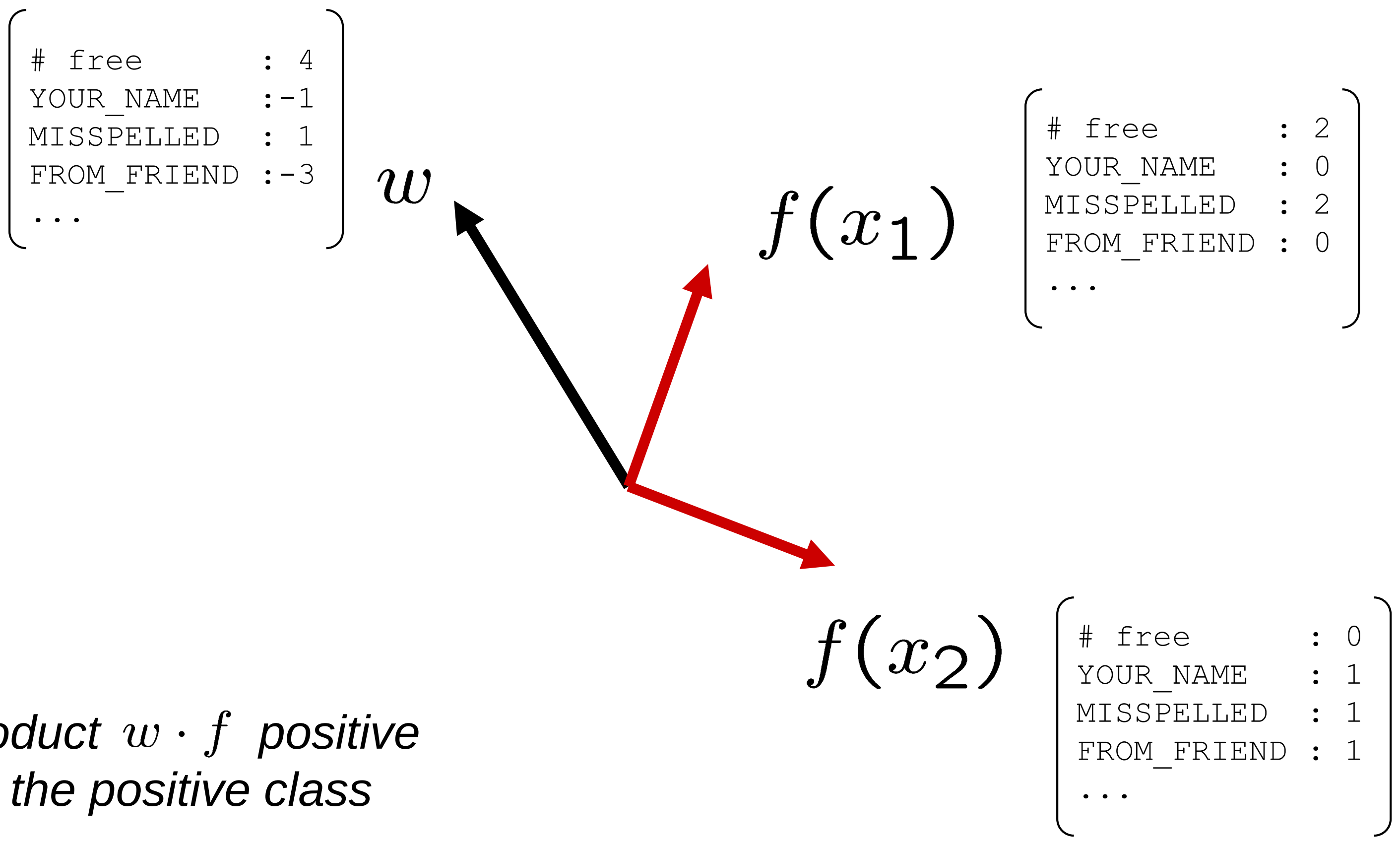
$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

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



Weights

- Binary case: compare features to a weight vector
- Learning: figure out the weight vector from examples



w:
```
# free       : 4
YOUR_NAME    :-1
MISSPELLED   : 1
FROM_FRIEND  :-3
...
```

$f(x_1)$:
```
# free       : 2
YOUR_NAME    : 0
MISSPELLED   : 2
FROM_FRIEND  : 0
...
```

$f(x_2)$:
```
# free       : 0
YOUR_NAME    : 1
MISSPELLED   : 1
FROM_FRIEND  : 1
...
```

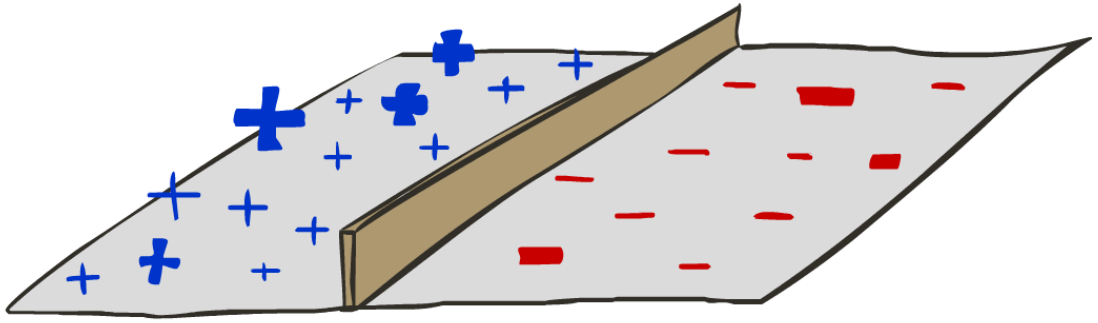
Dot product $w \cdot f$ *positive means the positive class*

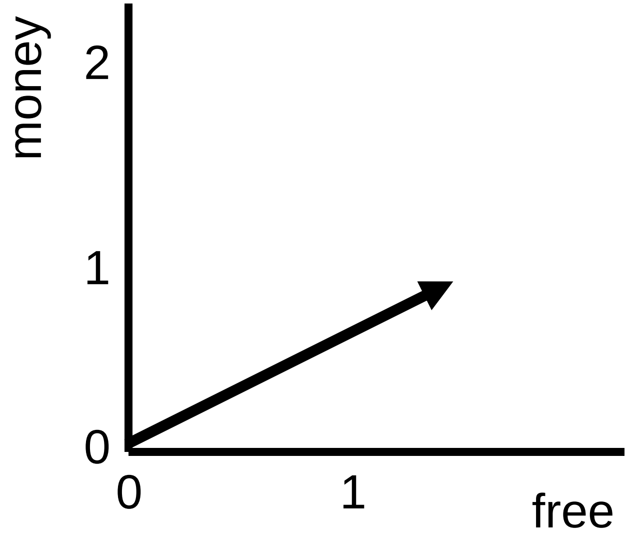
Binary Decision Rule

- In the space of feature vectors
  - Examples are points
  - Any weight vector is a hyperplane
  - One side corresponds to Y=+1
  - Other corresponds to Y=-1

w

```
BIAS  : -3
free  :  4
money :  2
...
```





Binary Decision Rule

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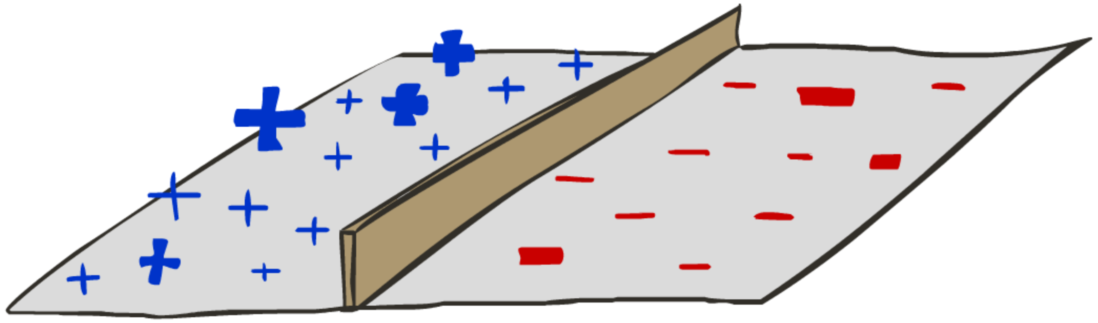
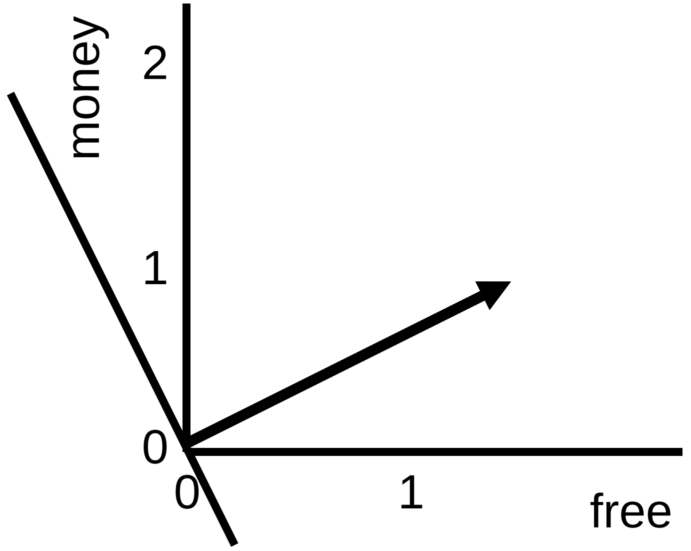


w

```
BIAS  : -3
free  :  4
money :  2
...
```



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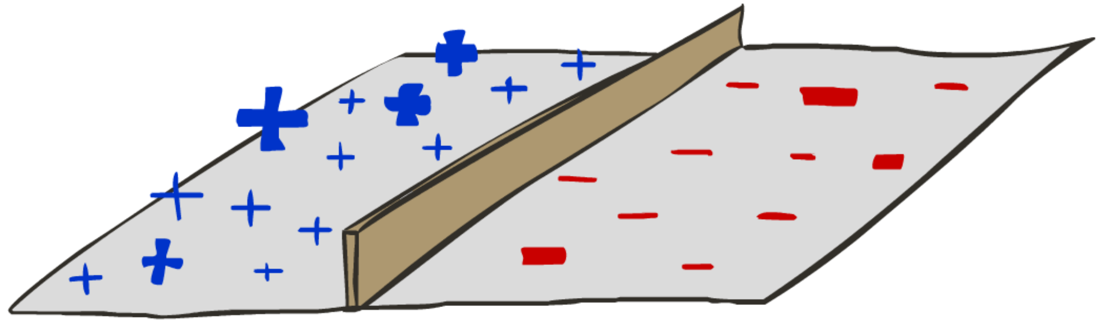
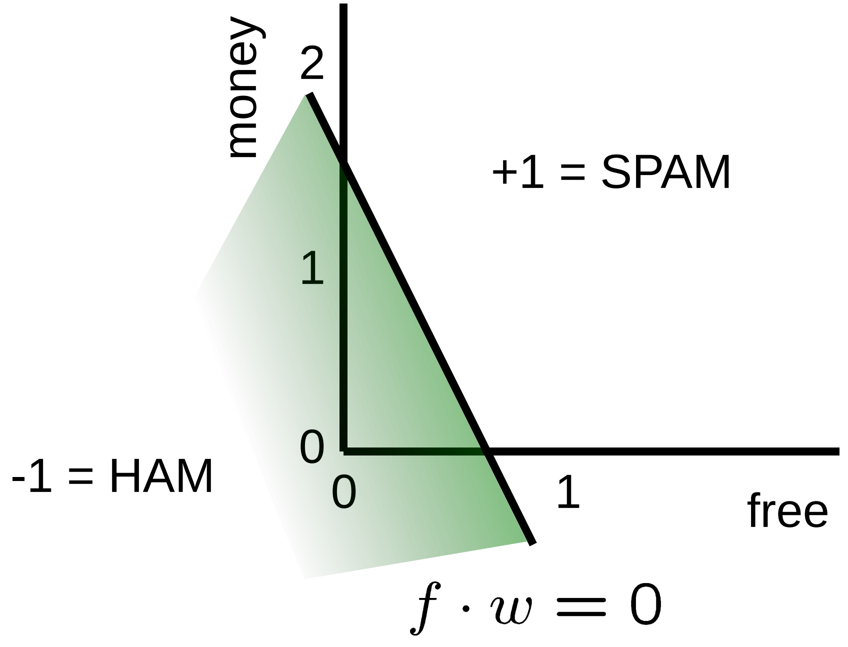


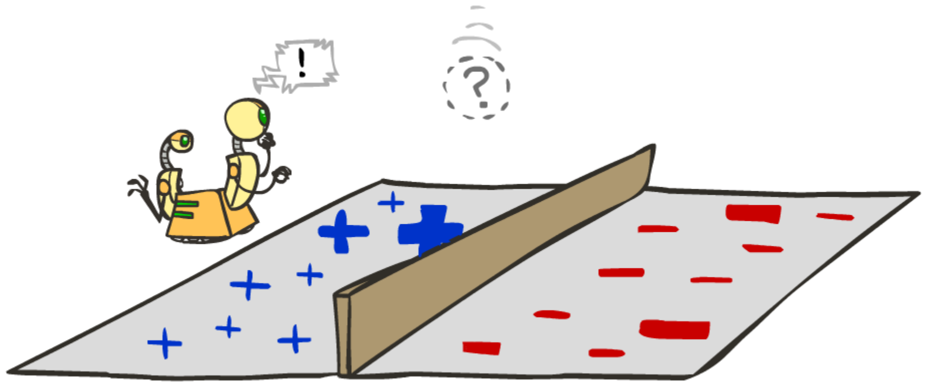
w

```
BIAS  : -3
free  :  4
money :  2
...
```

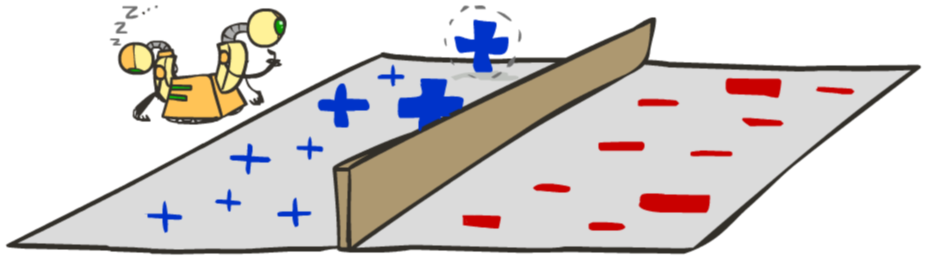


Learning: Binary Perceptron

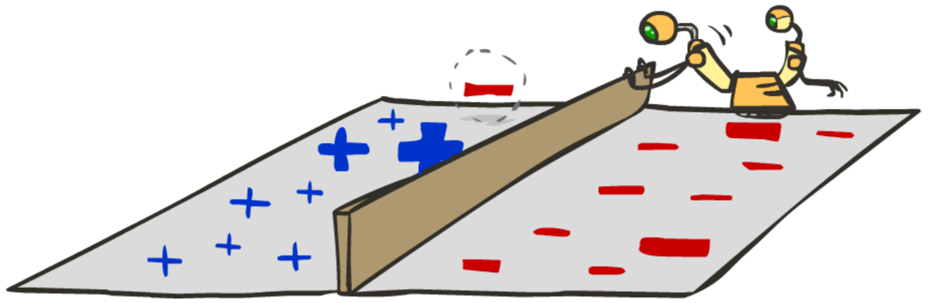
- Start with weights = 0
- For each training instance:
  - Classify with current weights



  - If correct (i.e., y=y*), no change!



  - If wrong: adjust the weight vector



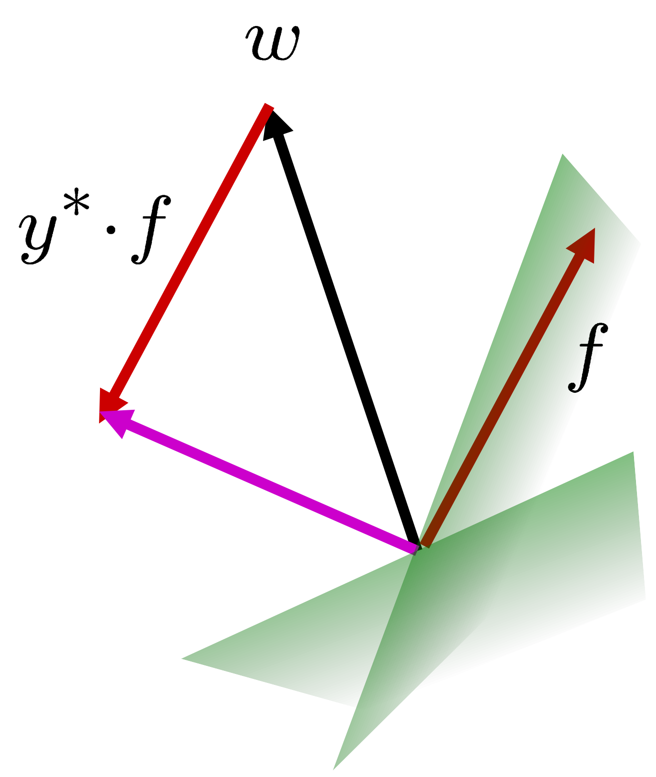
Learning: Binary Perceptron

- 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.

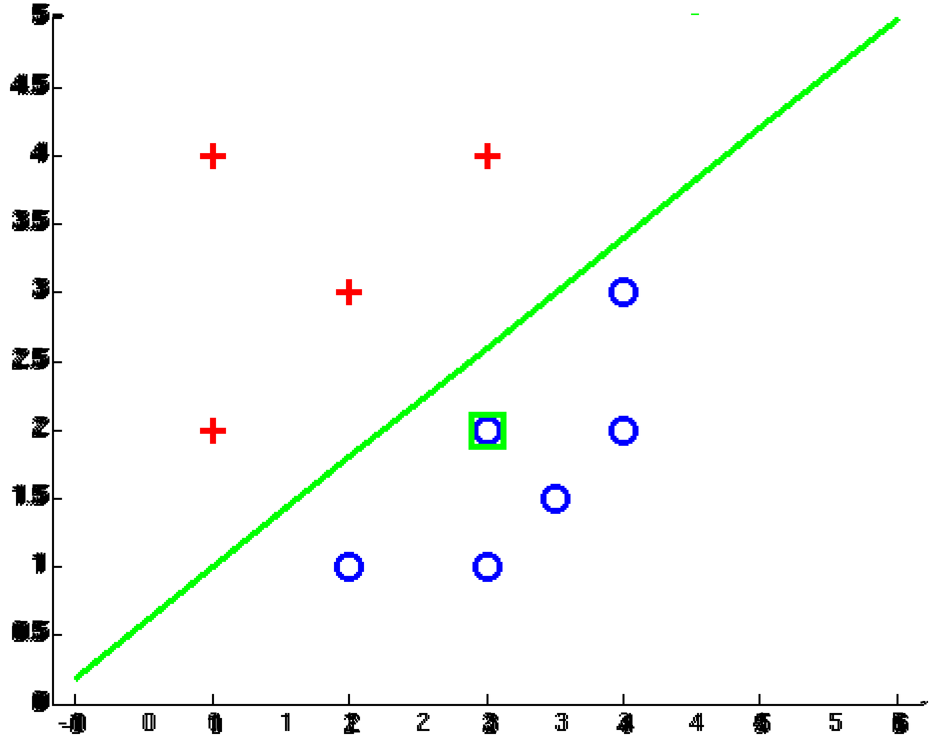
$$w = w + y^* \cdot f$$



Before: *w f*
After*: wf + y*f f*
f f >=0

Examples: Perceptron

- Separable Case

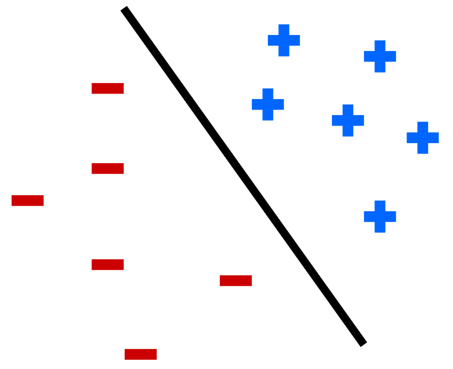


Properties of Perceptrons

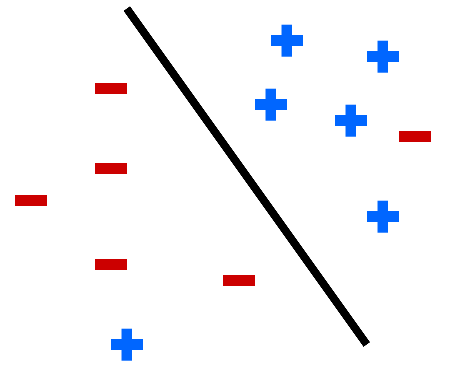
- Separability: true if some parameters get the training set perfectly correct
- Convergence: if the training is separable, perceptron will eventually converge (binary case)
- Mistake Bound: the maximum number of mistakes (binary case) related to the *margin* or degree of separability

$$\text{mistakes} < \frac{k}{\delta^2}$$

Separable

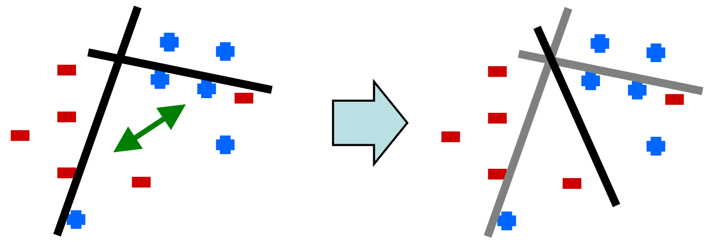


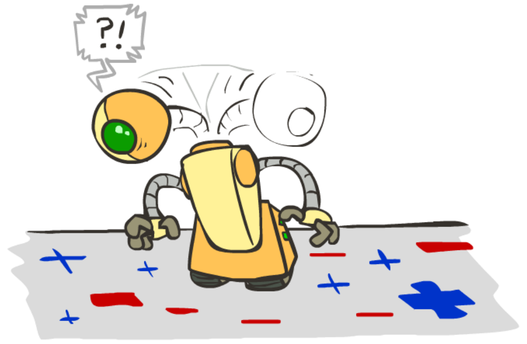
Non-Separable



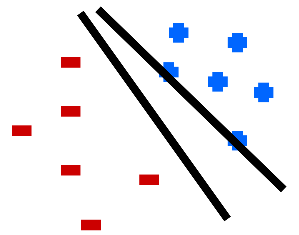
Problems with the Perceptron

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

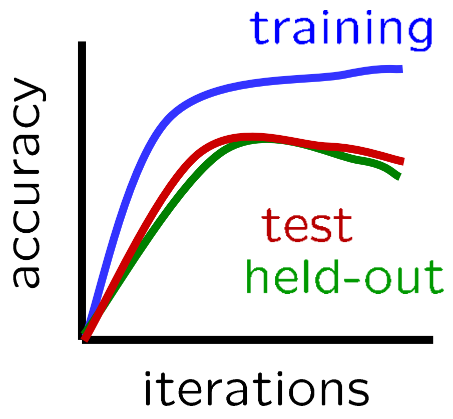


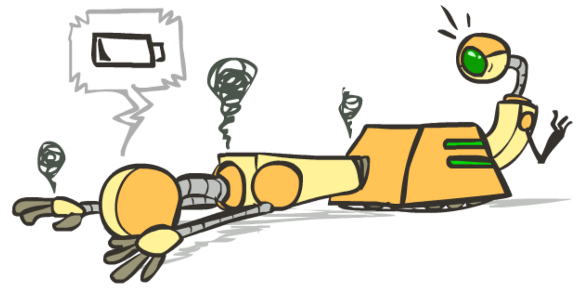


- Mediocre generalization: finds a "barely" separating solution

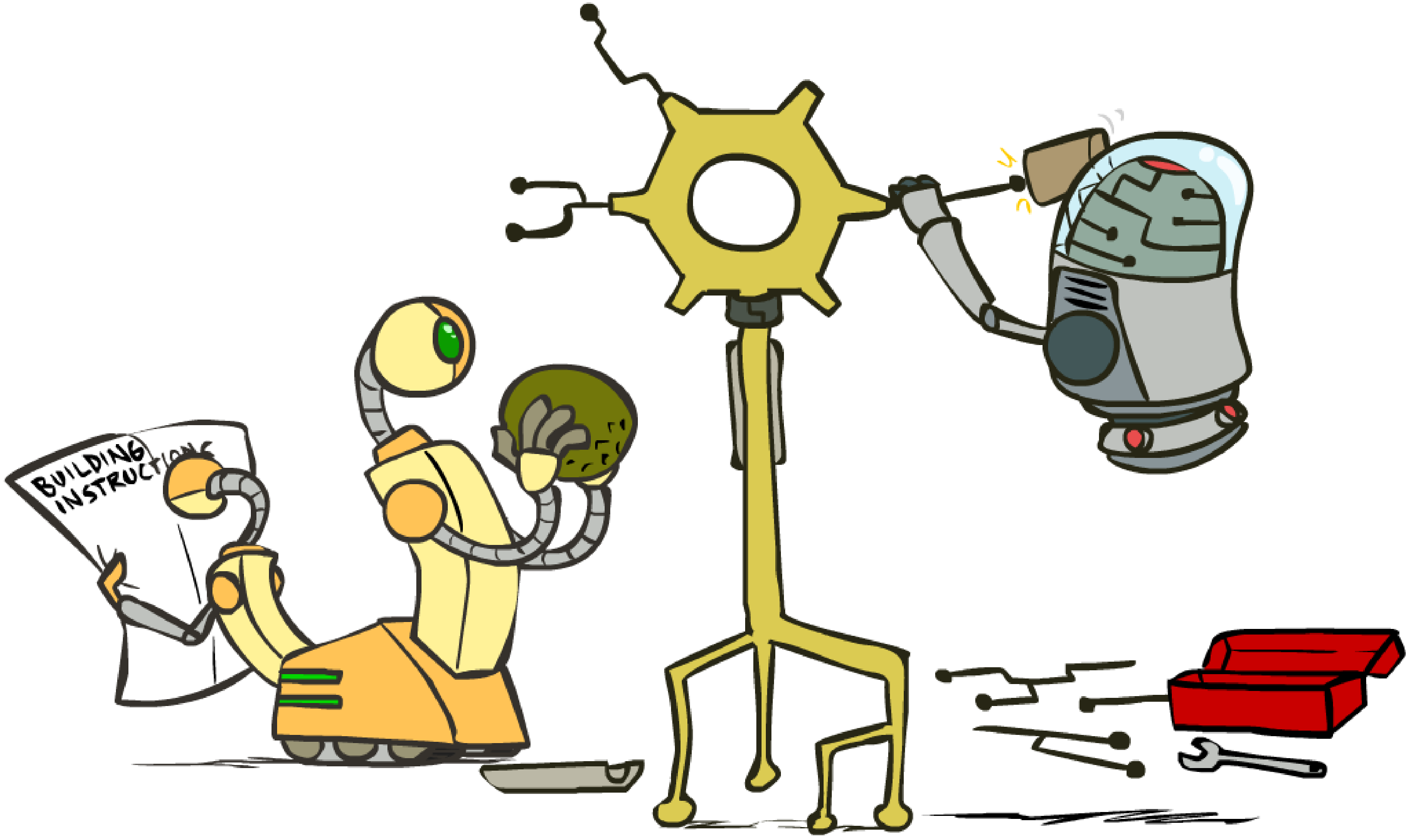


- Overtraining: test / held-out accuracy usually rises, then falls
  - Overtraining is a kind of overfitting



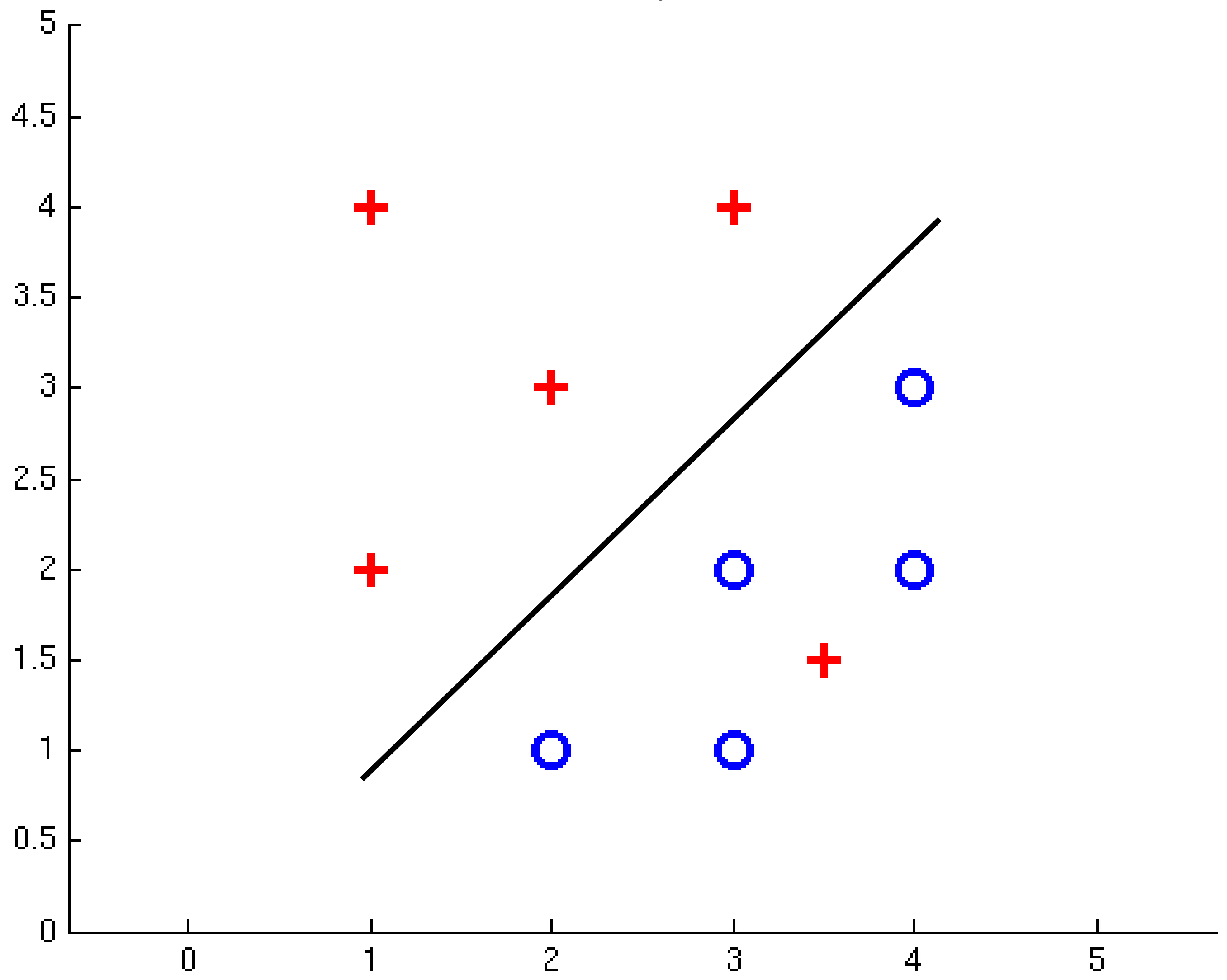


Improving the Perceptron

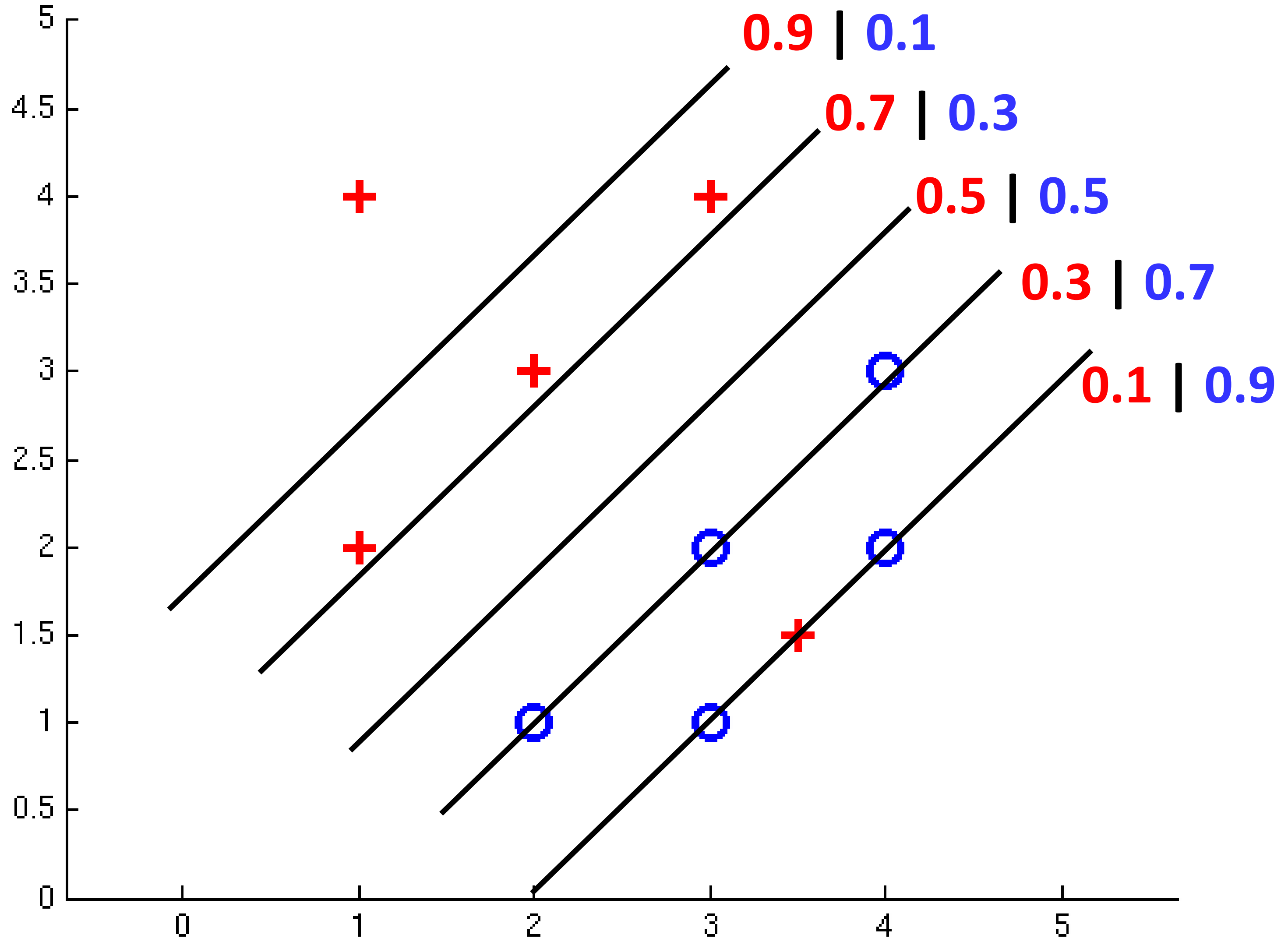


Non-Separable Case: Deterministic Decision

Even the best linear boundary makes at least one mistake



Non-Separable Case: Probabilistic Decision

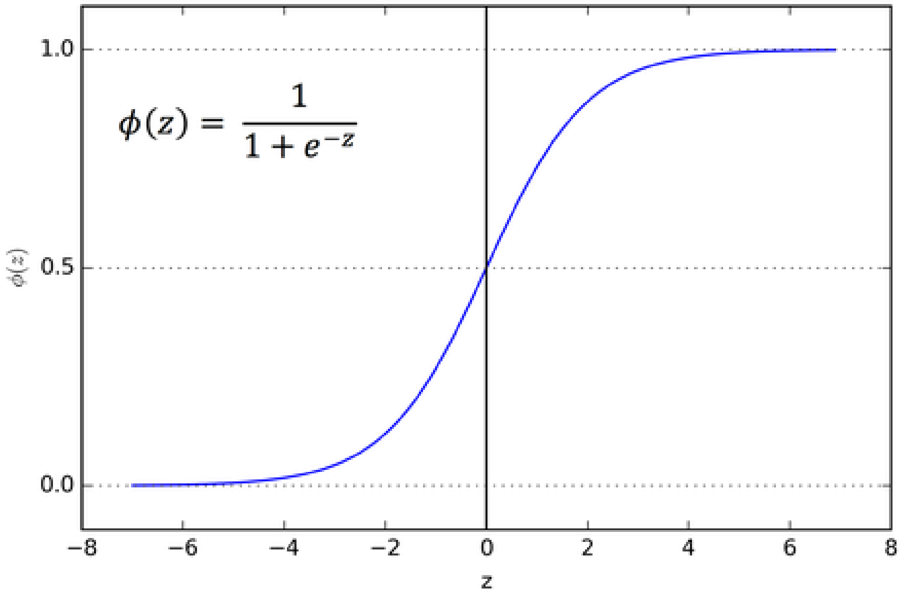


How to get probabilistic decisions?

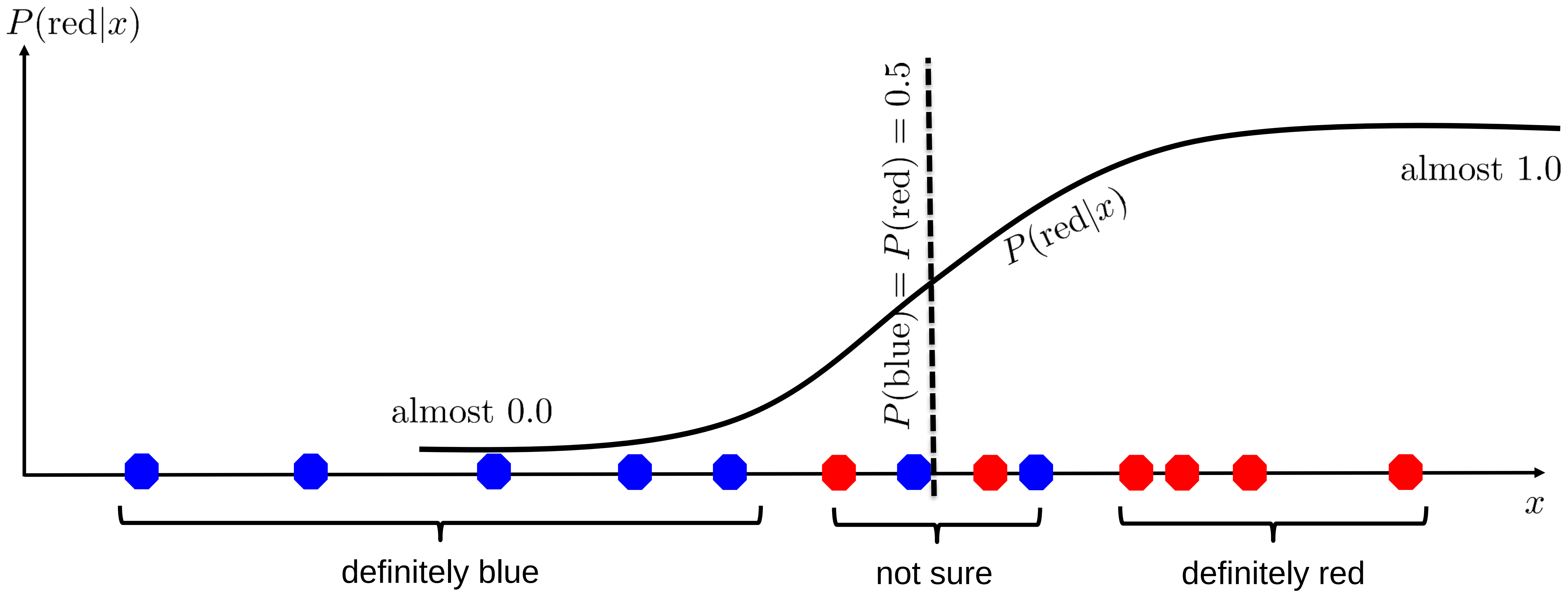
- Perceptron scoring: $z = w \cdot f(x)$
- If $z = w \cdot f(x)$ very positive → want probability going to 1
- If $z = w \cdot f(x)$ very negative → want probability going to 0

- Sigmoid function

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



A 1D Example



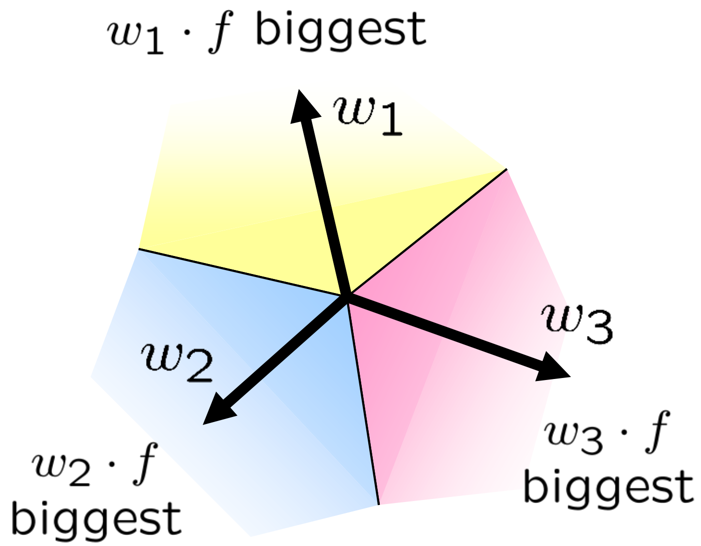
$$P(\text{red}|x) = \frac{e^{w_{\text{red}} \cdot x}}{e^{w_{\text{red}} \cdot x} + e^{w_{\text{blue}} \cdot x}}$$

probability increases exponentially as we move away from boundary

normalizer

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

Optimization

- i.e., how do we solve:

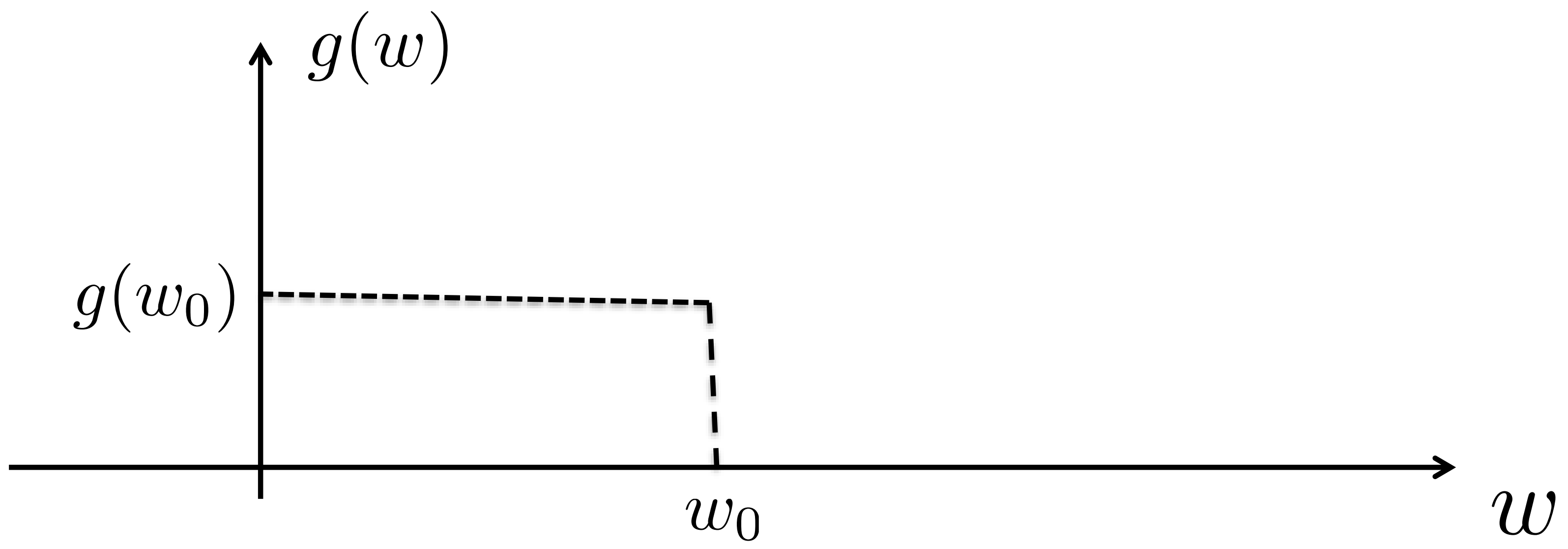
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

Hill Climbing

- 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?

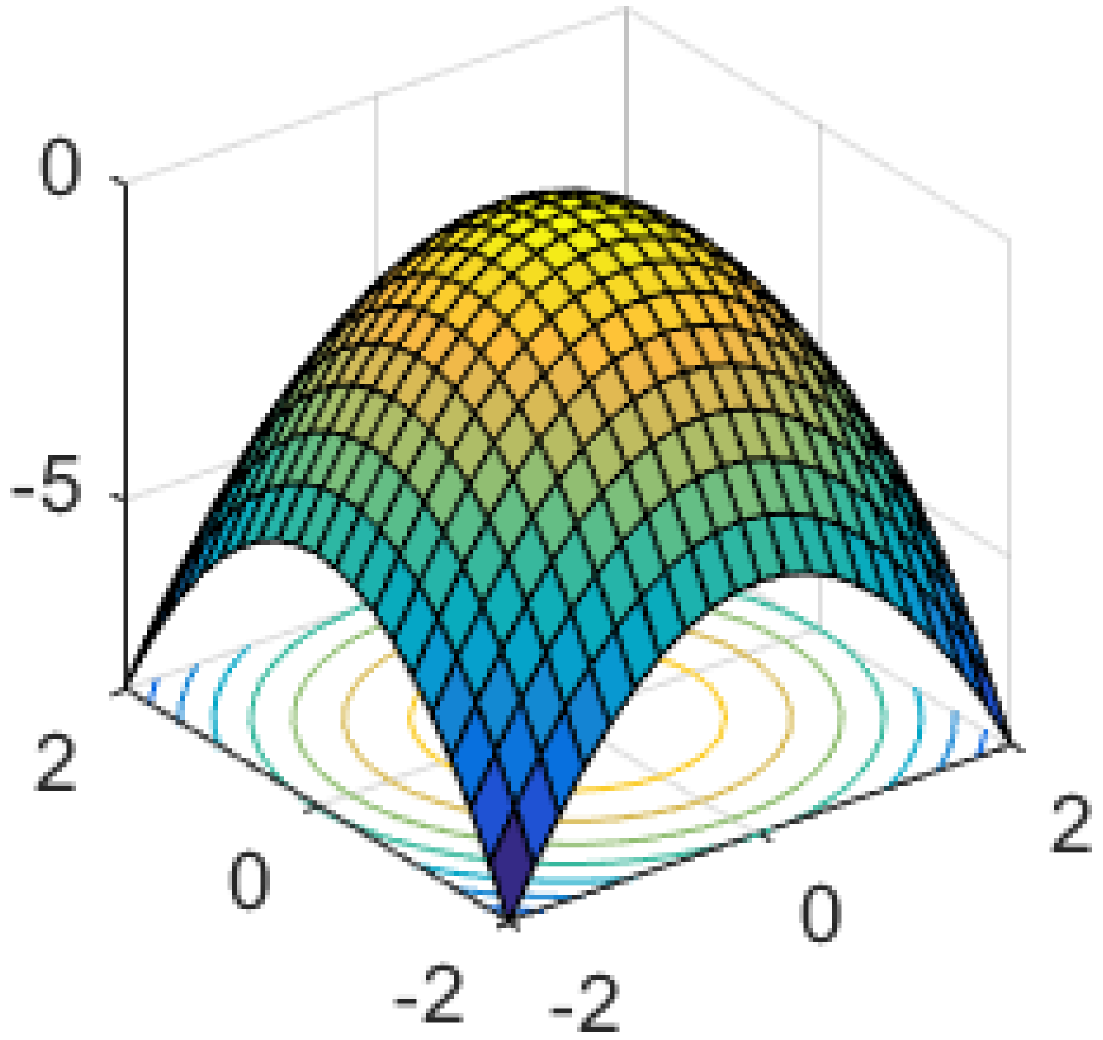
1-D Optimization



- Could evaluate $g(w_0 + h)$ 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



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

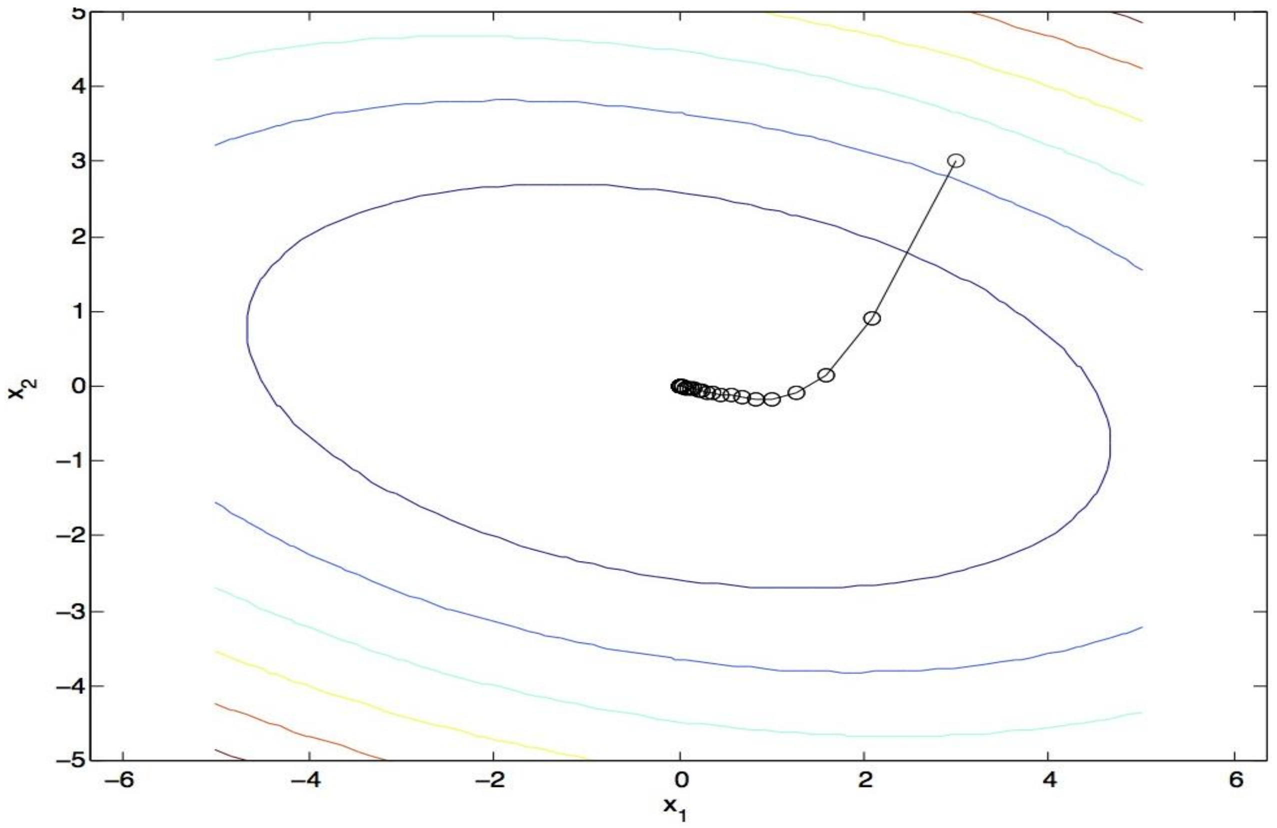
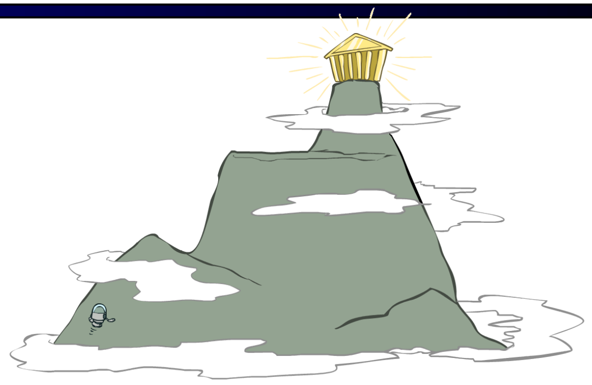


Figure source: Mathworks

What is the Steepest Direction?



$$\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} \quad g(w+\Delta)$$

- First-Order Taylor Expansion: $$g(w+\Delta) \approx g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$$
- Steepest Ascent Direction: $$\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} \quad g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$$
- Recall: $\max_{\Delta:\|\Delta\|\leq\varepsilon} \Delta^\top a \quad \rightarrow \quad \Delta = \varepsilon\frac{a}{\|a\|}$
- Hence, solution: $\Delta = \varepsilon\frac{\nabla g}{\|\nabla g\|}$ **Gradient direction = steepest direction!** $\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \end{bmatrix}$

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
  - Crude rule of thumb: update changes w about 0.1 – 1 %

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

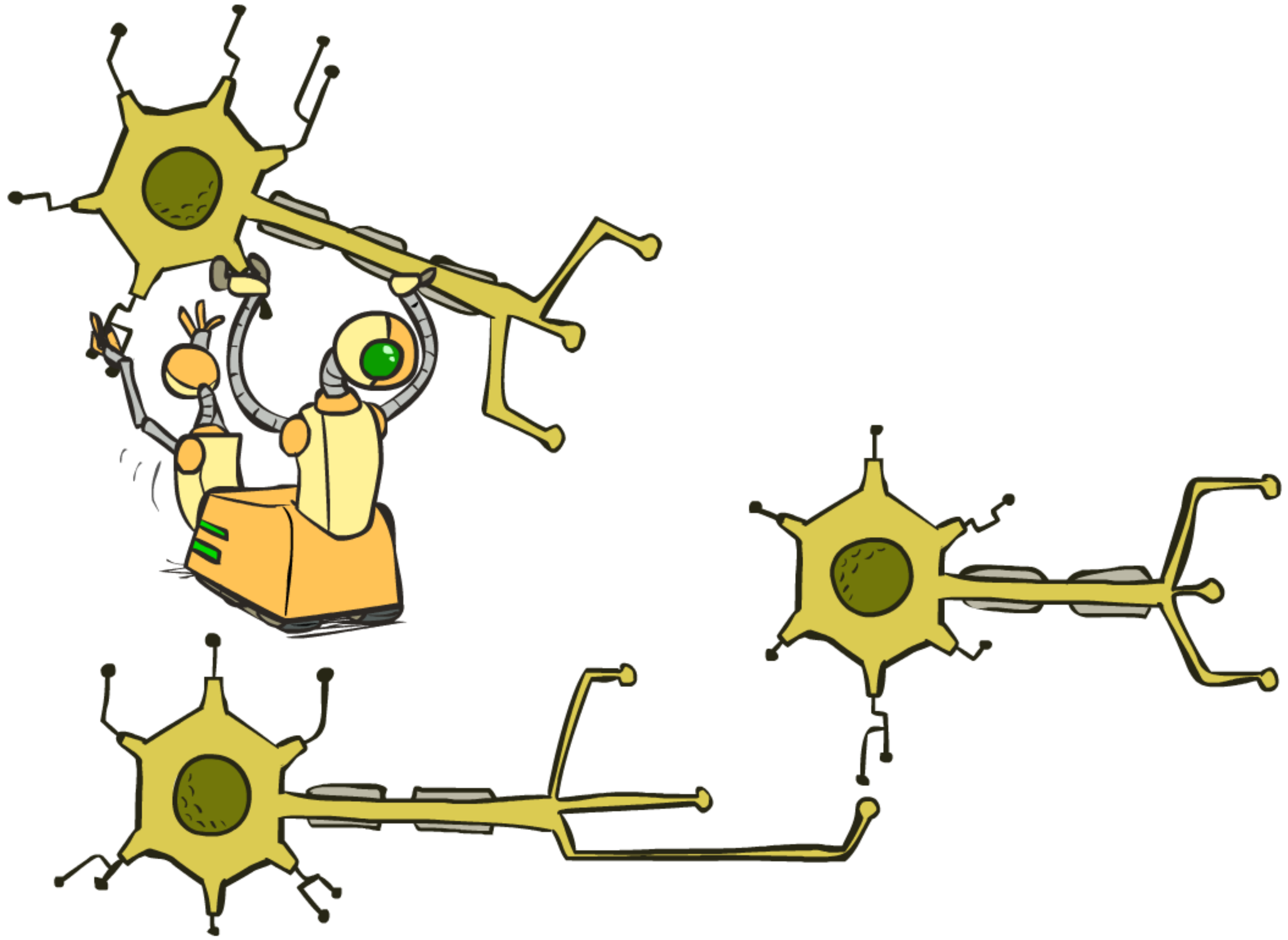
Mini-Batch Gradient Ascent on the Log Likelihood Objective

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

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

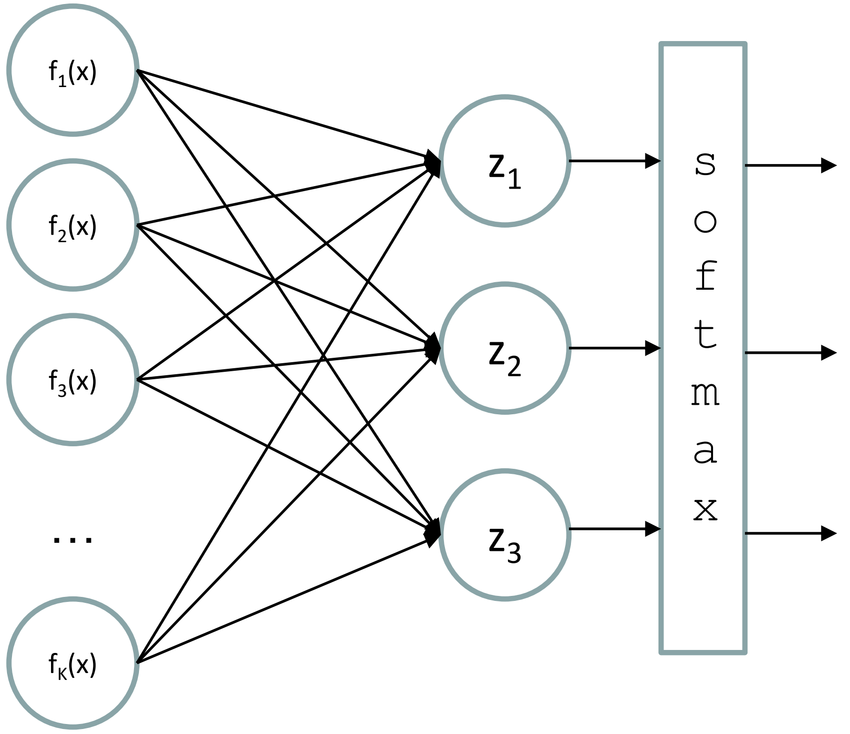
```
- init $w$
- for iter = 1, 2, …
    - pick random subset of training examples J
      $w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)}|x^{(j)}; w)$
```

Neural Networks



Multi-class Logistic Regression

- = special case of neural network

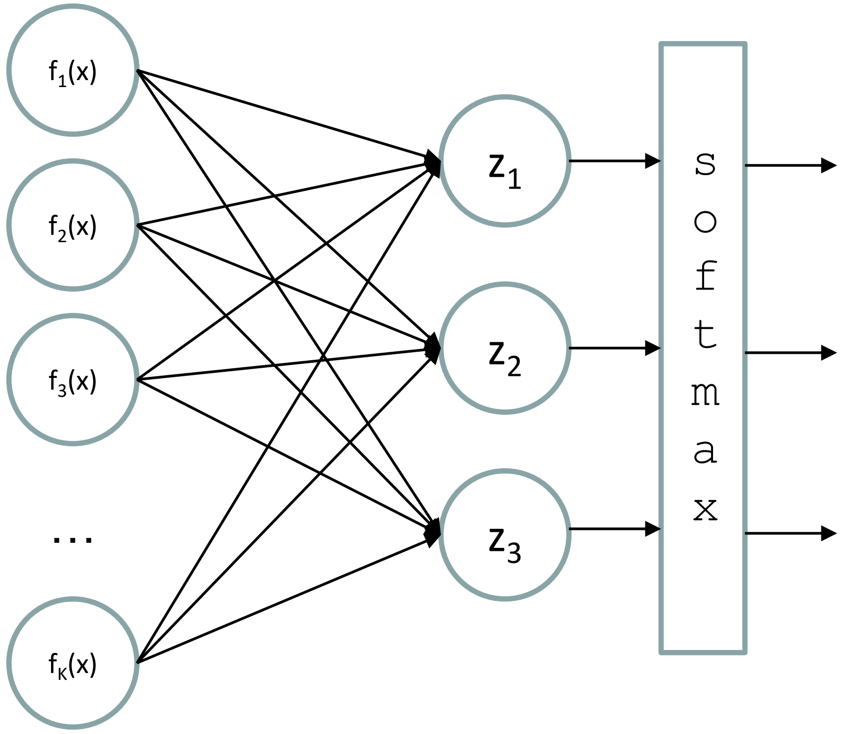


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

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

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

Deep Neural Network = Also learn the features!



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

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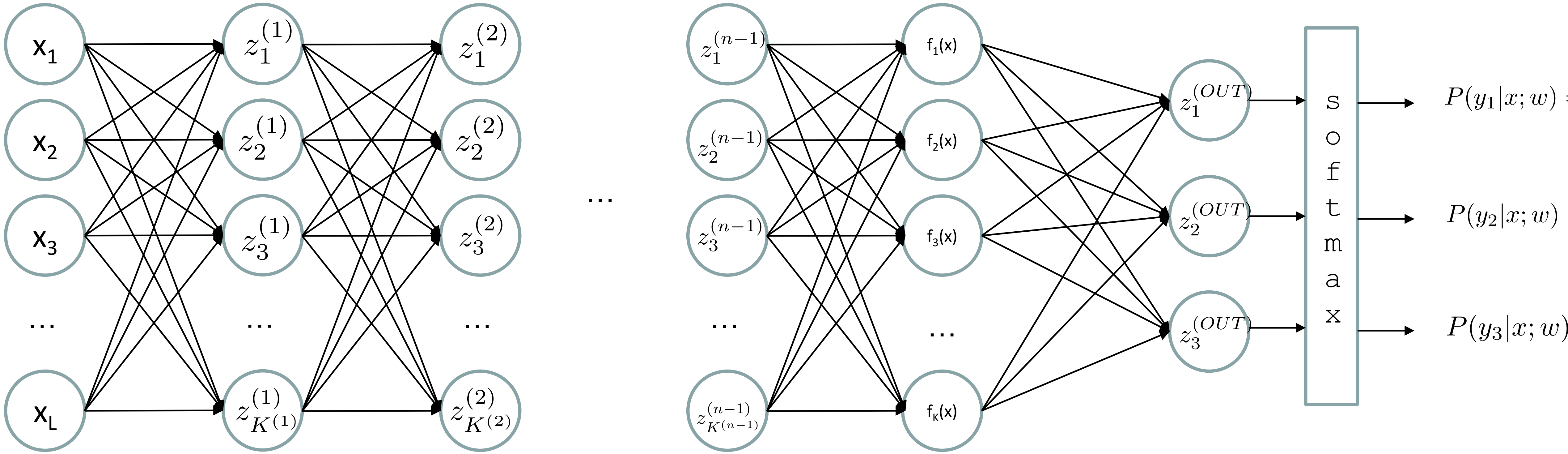
$$P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}}$$

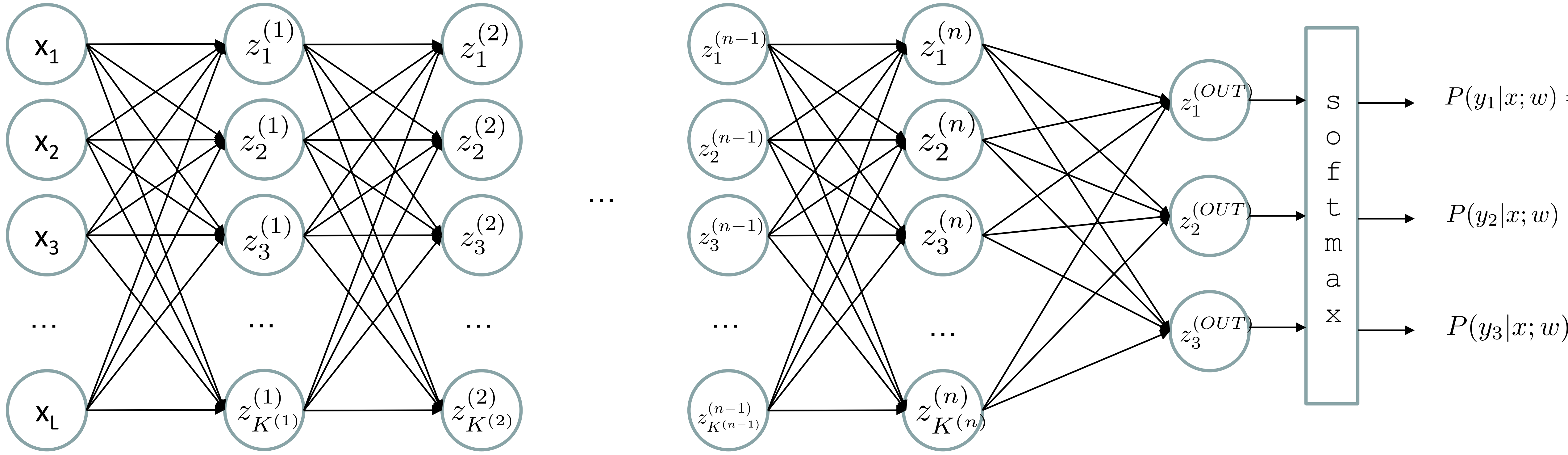
Deep Neural Network = Also learn the features!



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

g = nonlinear activation function

Deep Neural Network = Also learn the features!

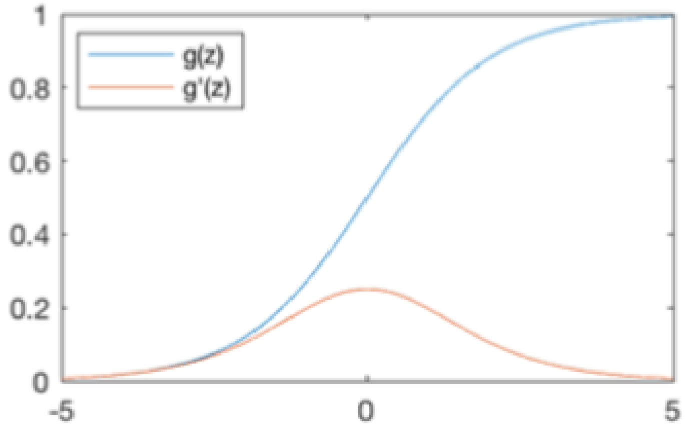


$$z_i^{(k)} = g(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

g = nonlinear activation function

Common Activation Functions

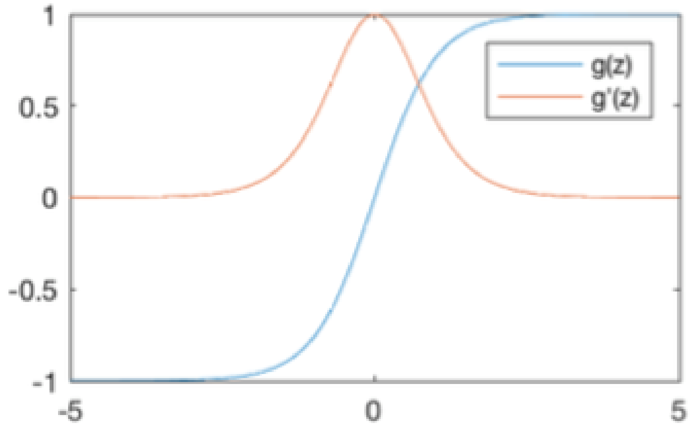
Sigmoid Function



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

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

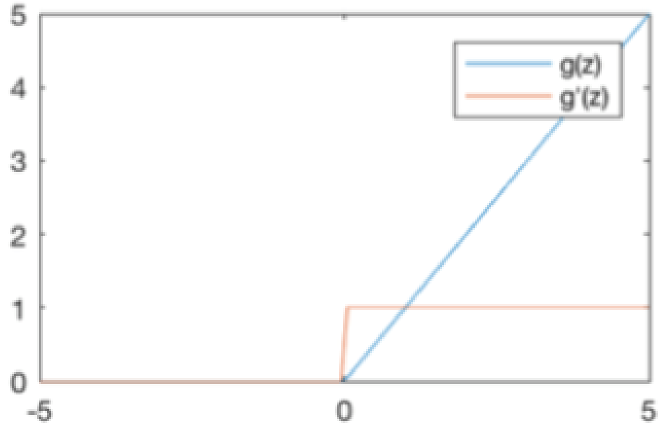
Hyperbolic Tangent



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

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

Rectified Linear Unit (ReLU)



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

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

[source: MIT 6.S191 introtodeeplearning.com]

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

How about computing all the derivatives?

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

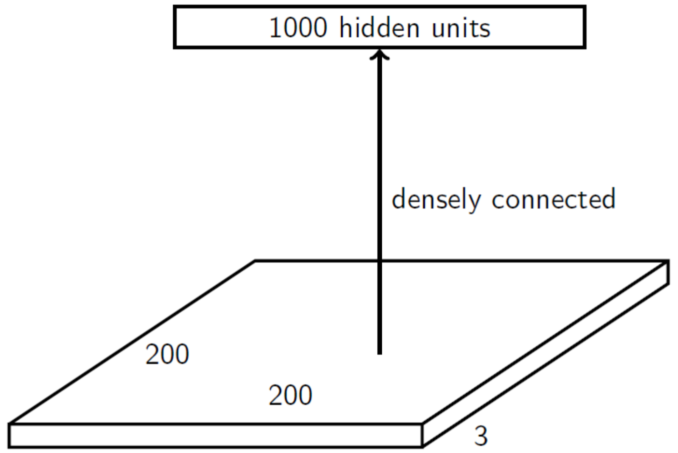
If $$f(x) = g(h(x))$$

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

→ **Derivatives can be computed by following well-defined procedures**

Motivation

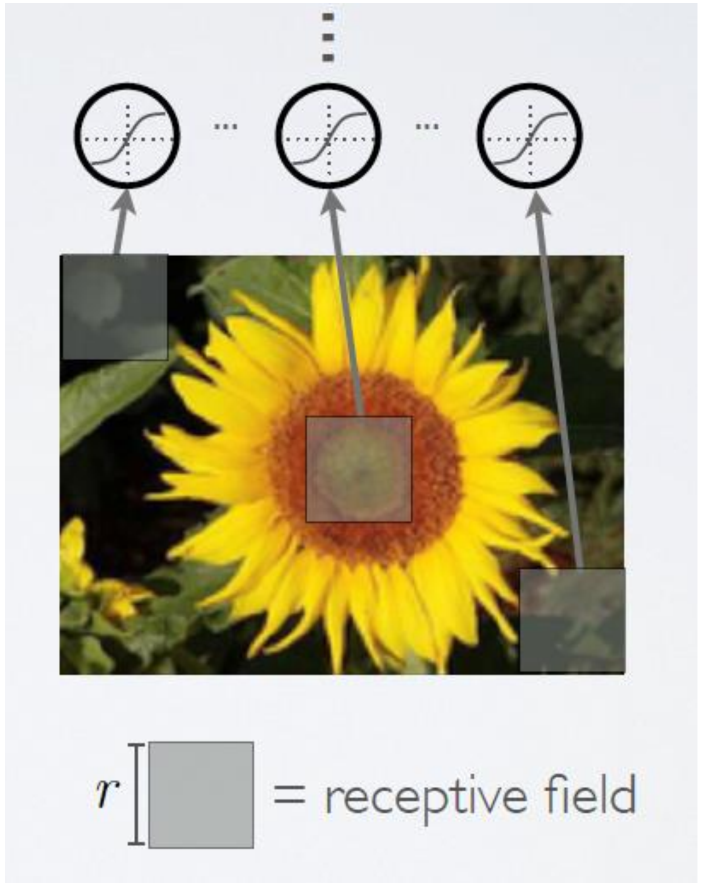
- Visual recognition
  - Suppose we aim to train a network that takes a 200x200 RGB image as input



  - What is the problem with have full connections in the first layer?
    - Too many parameters! 200x200x3x1000 = 120 million
    - What happens if the object in the image shifts a little?

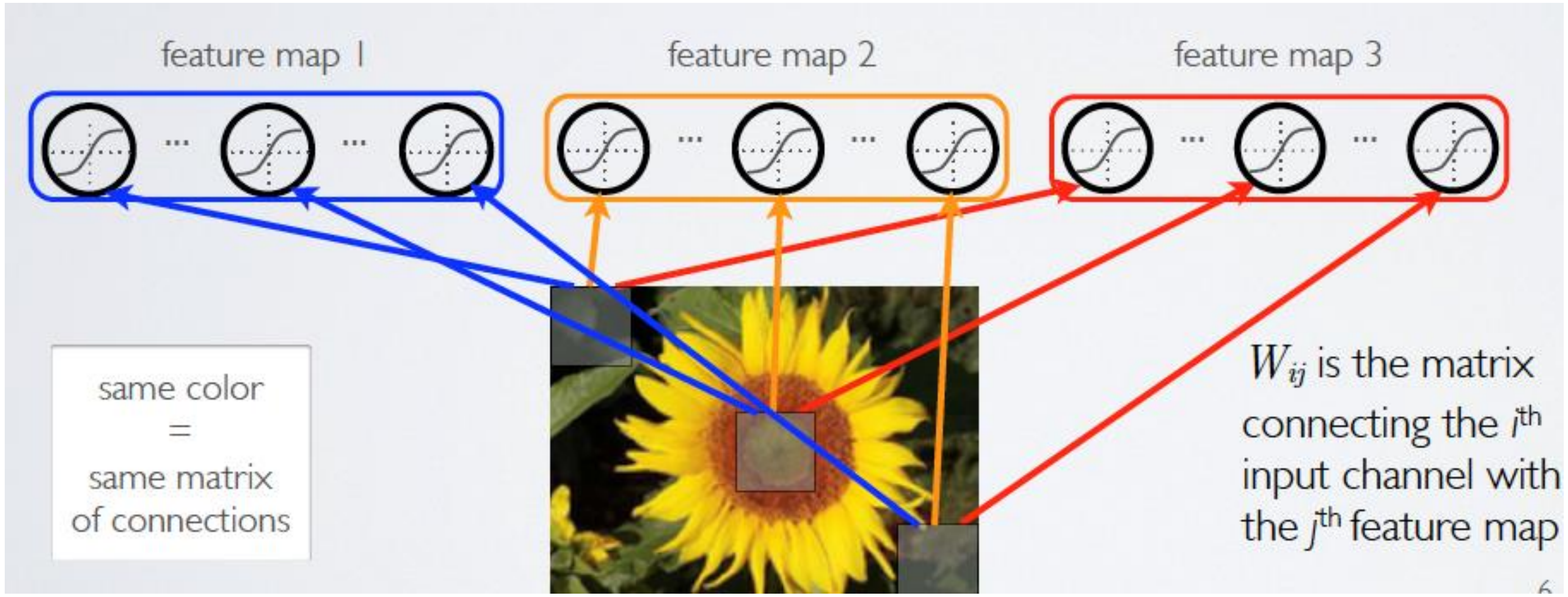
Overview of CNNs

- First idea: Use a local connectivity of hidden units
  - Each hidden unit is connected only to a subregion (patch) of the input image
  - Usually it is connected to all channels
  - Each neuron has a local receptive field



Overview of CNNs

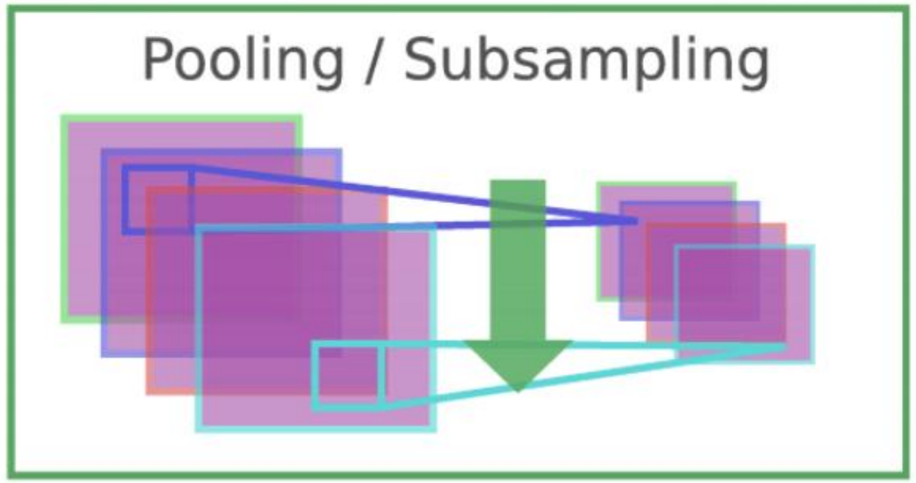
- Second idea: share weights across certain units
  - Units organized into the same “feature map” share weight parameters
  - Hidden units within a feature map cover different positions in the image



feature map 1
feature map 2
feature map 3
same color = same matrix of connections
W_{ij} is the matrix connecting the i^{th} input channel with the j^{th} feature map
6

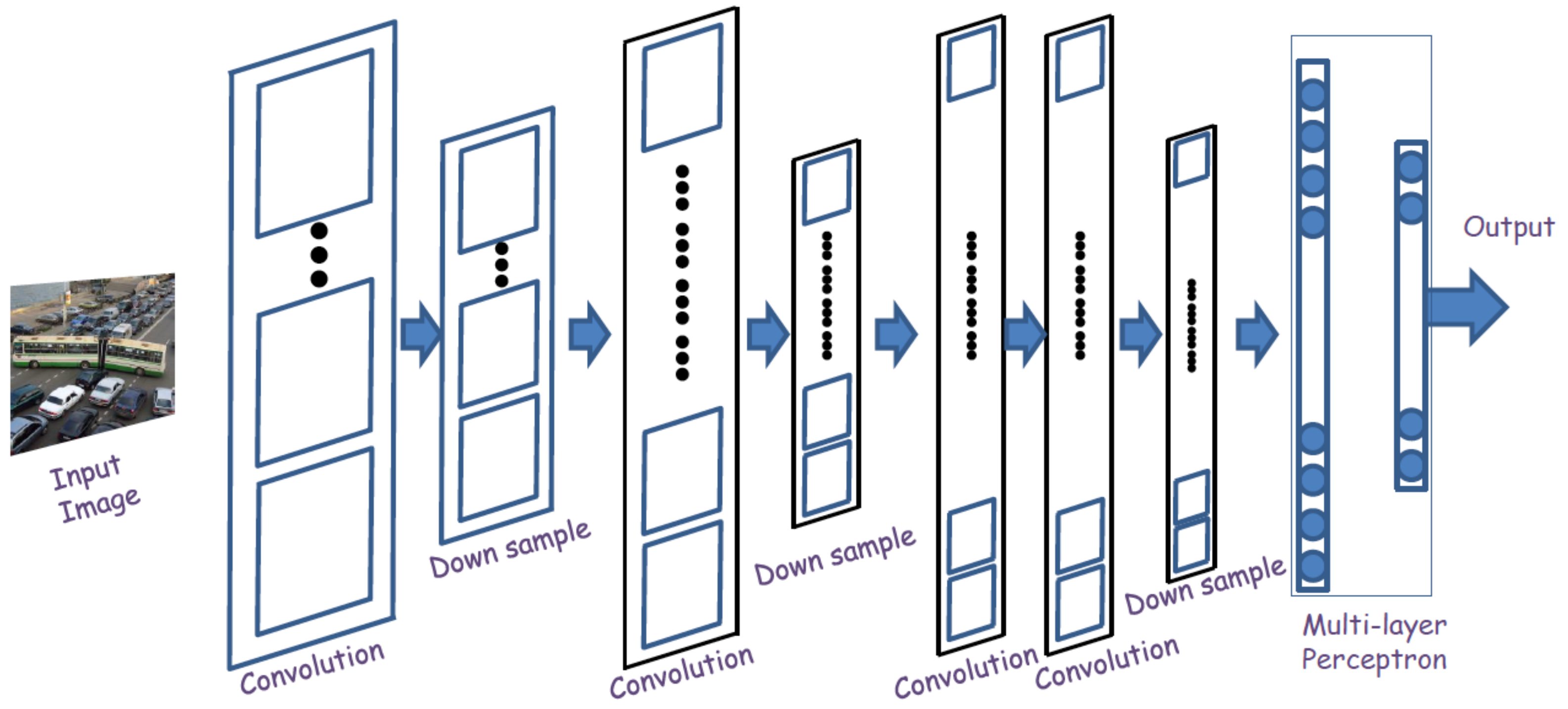
Overview of CNNs

- Third idea: pool hidden units in the same neighborhood
  - Averaging or Discarding location information in a small region
  - Robust toward small deformations in object shapes by ignoring details.



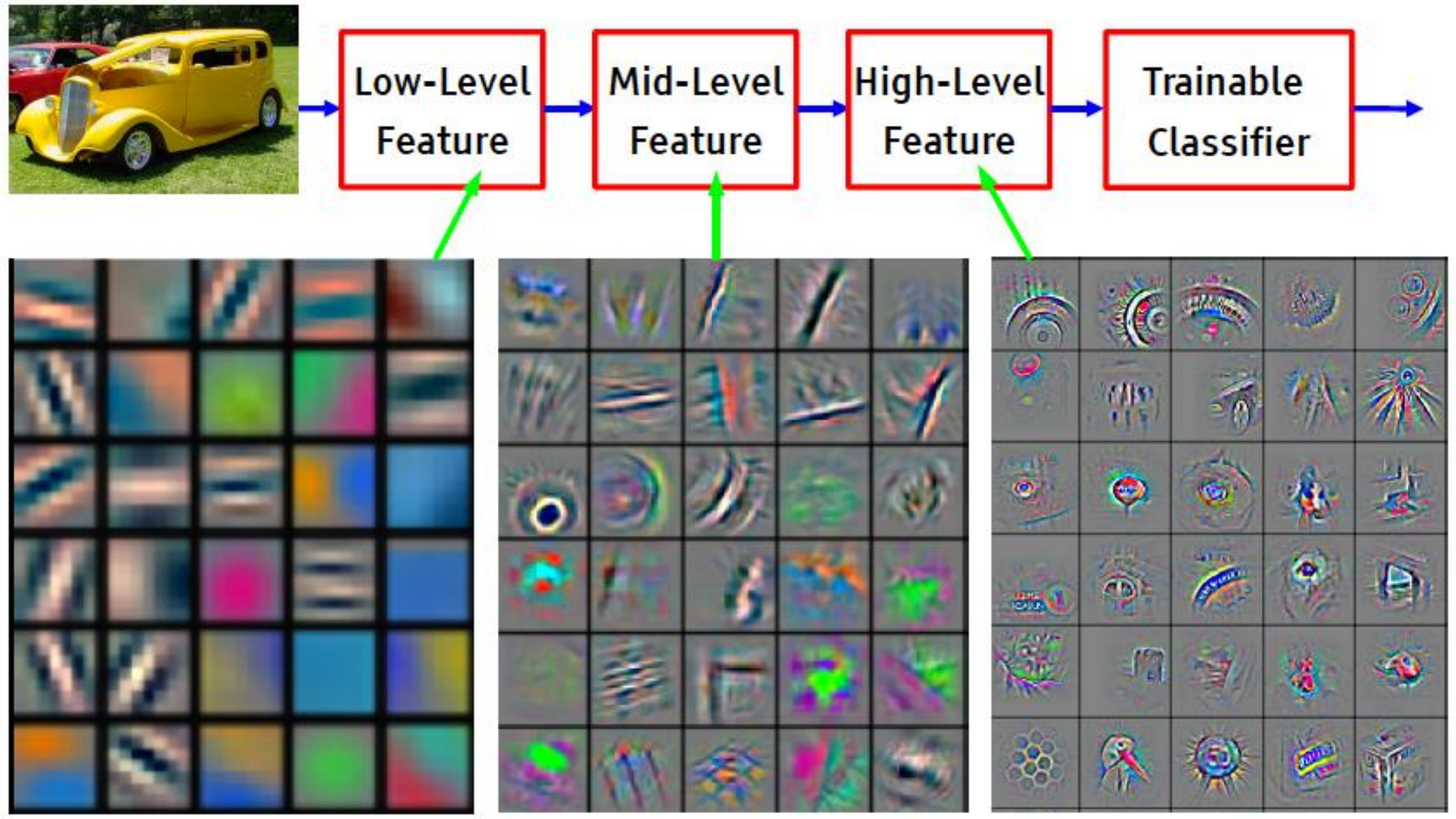
Overview of CNNs

- Fourth idea: Interleaving feature extraction and pooling operations
  - Extracting abstract, compositional features for representing semantic object classes



Overview of CNNs

- Artificial visual pathway: from images to semantic concepts (Representation learning)

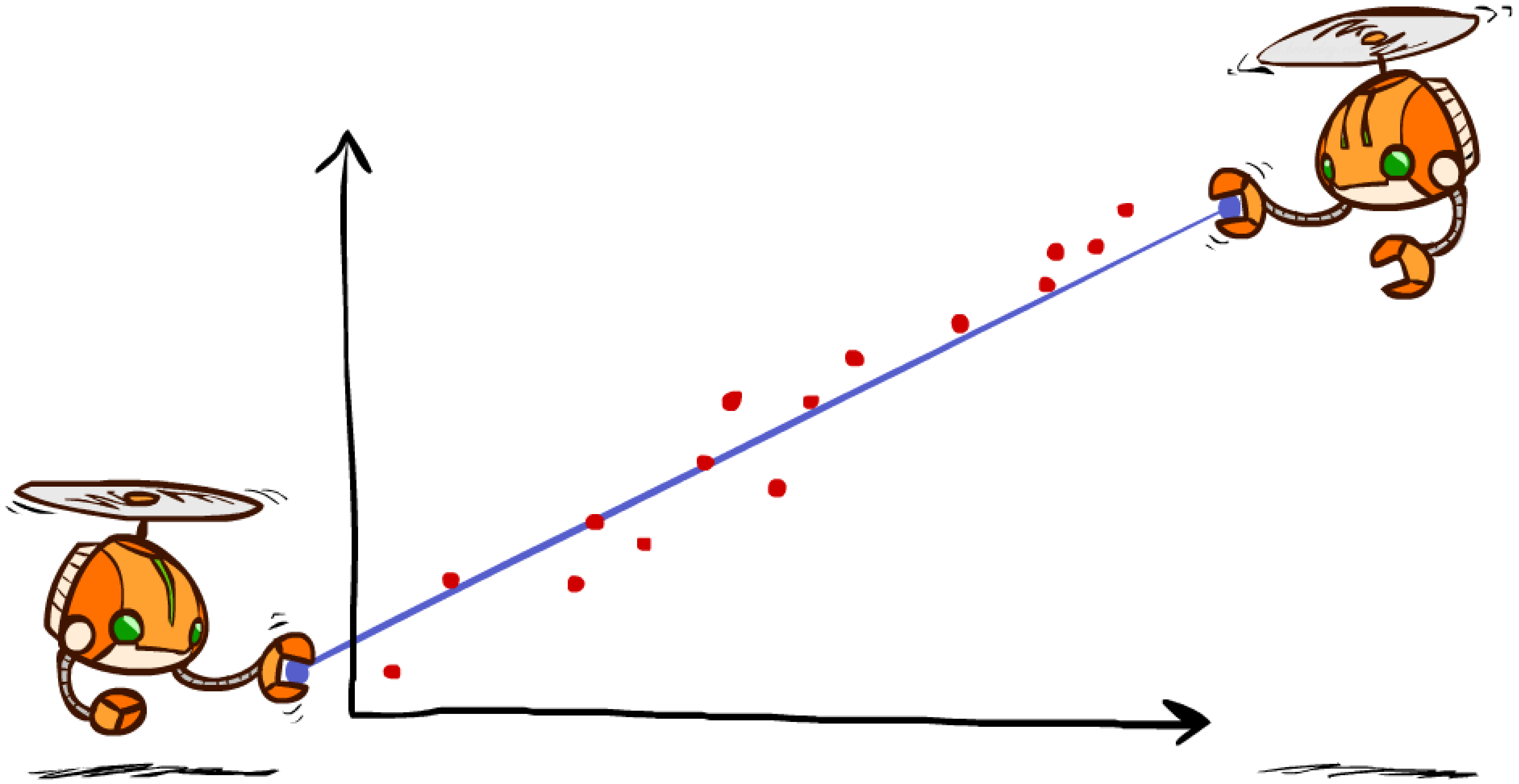


Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

More classification methods

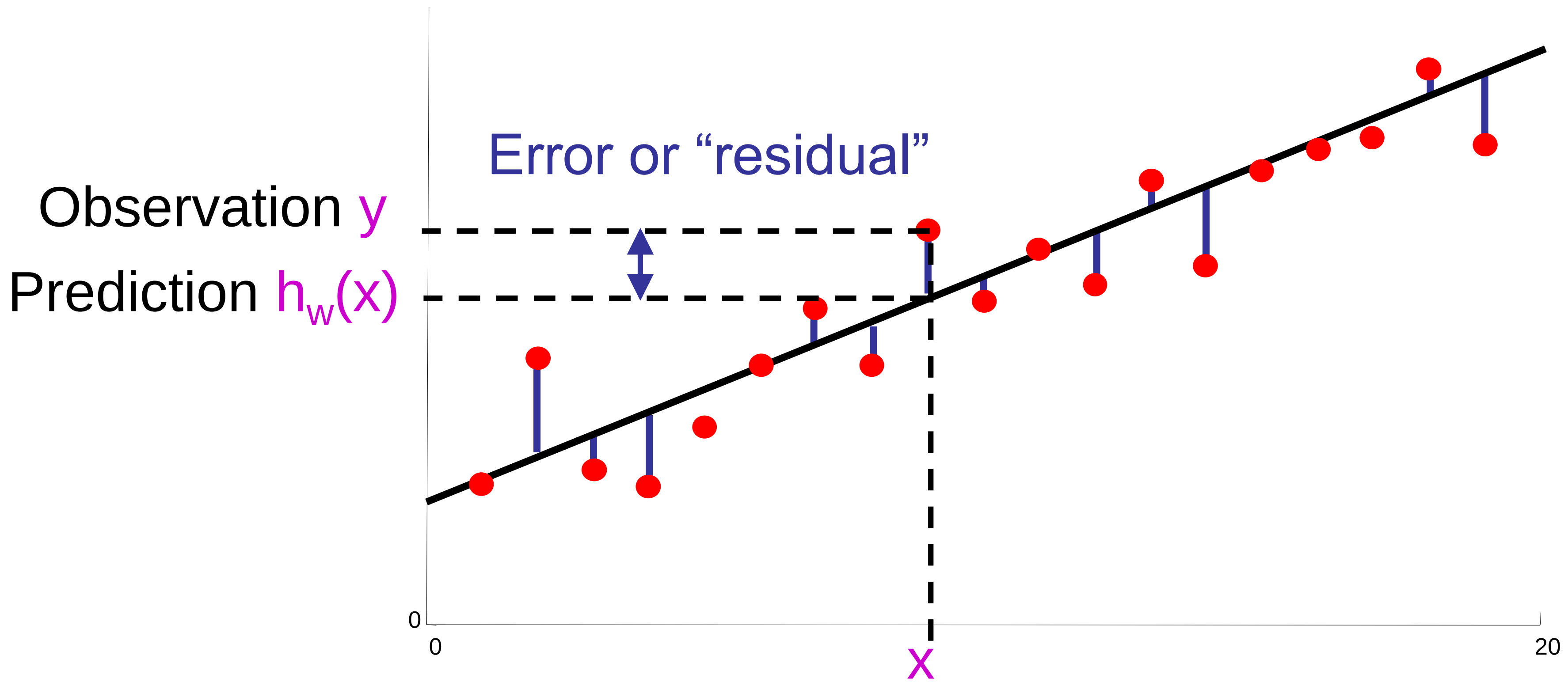
- Naive Bayes
- Perceptron / Neural networks
- Decision trees / Random forest
- Support Vector Machines
- Nearest neighbors
- Model ensembles: bagging, boosting, etc.
- ……

Regression



Linear Regression

Prediction: $h_w(x) = w_0 + w_1x$



Error on one instance: $|y – h_w(x)|$

Least squares: Minimizing squared error

- L2 loss function: sum of squared errors over all examples

$$L(\boldsymbol{w}) = \sum_i \left(y_i - h_w(\boldsymbol{x}_i)\right)^2 = \sum_i (y_i - \boldsymbol{w}^T \boldsymbol{x}_i)^2$$

- We want the weights w* that minimize loss
- Analytical solution: at w* the derivative of loss w.r.t. each weight is zero
  - **X** is the data matrix (all the data, one example per row); **y** is the vector of labels
  - $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

Regularized Regression

- Overfitting is also possible in regression
  - Extreme case: *n* features, *n* training examples
- Regularization can be used to alleviate overfitting

- LASSO (Least Absolute Shrinkage and Selection Operator)

$$L(\boldsymbol{w}) = \sum_i (y_i - \boldsymbol{w}^T \boldsymbol{x}_i)^2 + \lambda \sum_k |w_k|$$

- Ridge Regression

$$L(\boldsymbol{w}) = \sum_i (y_i - \boldsymbol{w}^T \boldsymbol{x}_i)^2 + \lambda \sum_k w_k^2$$