CS 188: Artificial Intelligence

Machine Learning

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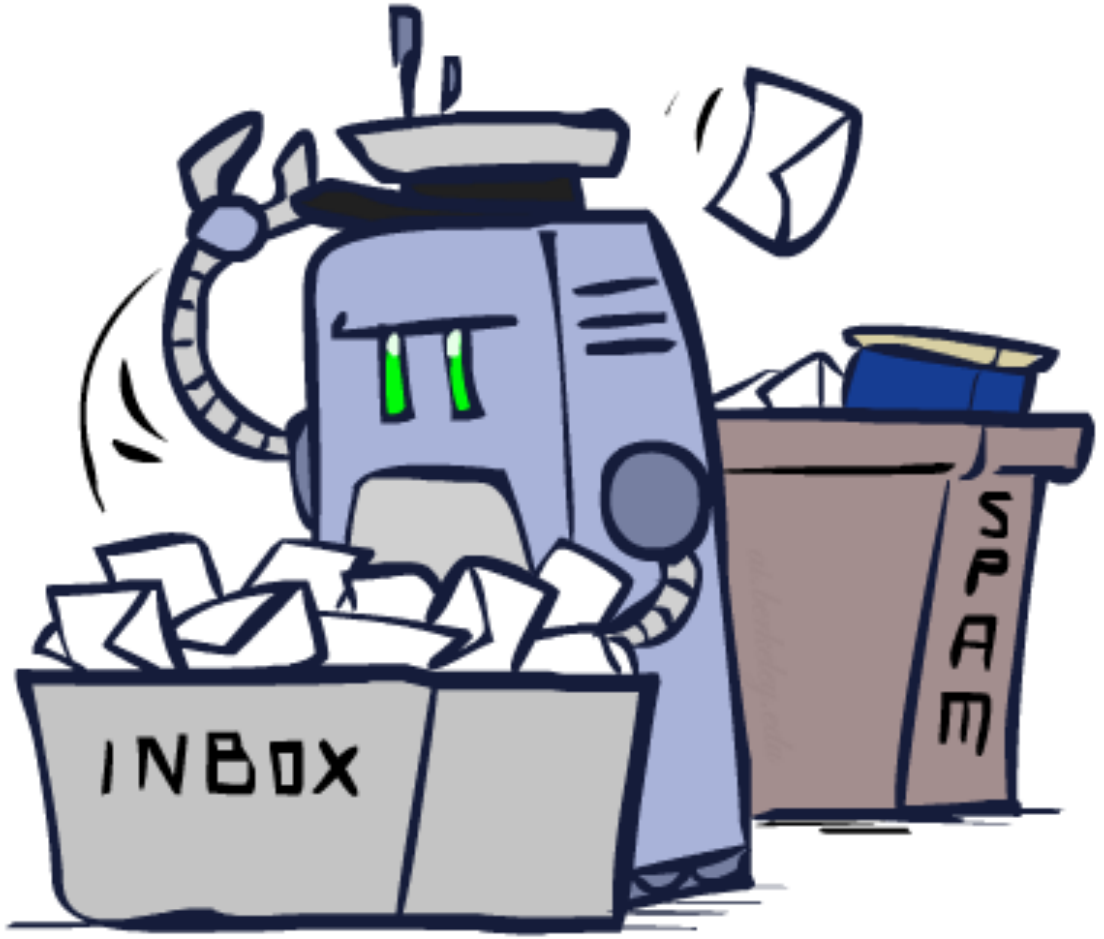
[Slides based on those by Nicholas Tomlin, Dan Klein and Pieter Abbeel for CS188 Intro to AI at UC Berkeley. CS188 materials are available at http://ai.berkeley.edu.]

Machine Learning

- Up until now: how use a model to make optimal decisions
- Machine learning: how to acquire a model from data / experience
  - Learning parameters (e.g. probabilities)
  - Learning structure (e.g. BN graphs)
  - Learning hidden concepts (e.g. clustering, neural nets)
- Today: model-based classification with Naive Bayes

Classification



Example: Spam Filter

- Input: an email
- Output: spam/ham

- Setup:
  - Get a large collection of example emails, each labeled "spam" or "ham"
  - Note: someone has to hand label all this data!
  - Want to learn to predict labels of new, future emails

- Features: The attributes used to make the ham / spam decision
  - Words: FREE!
  - Text Patterns: $dd, CAPS
  - Non-text: SenderInContacts, WidelyBroadcast
  - …

Dear Sir.

First, I must solicit your confidence in this transaction, this is by virture of its nature as being utterly confidencial and top secret. …

TO BE REMOVED FROM FUTURE MAILINGS, SIMPLY REPLY TO THIS MESSAGE AND PUT "REMOVE" IN THE SUBJECT.

99 MILLION EMAIL ADDRESSES
FOR ONLY $99

Ok, Iknow this is blatantly OT but I'm beginning to go insane. Had an old Dell Dimension XPS sitting in the corner and decided to put it to use, I know it was working pre being stuck in the corner, but when I plugged it in, hit the power nothing happened.

Example: Digit Recognition

- Input: images / pixel grids
- Output: a digit 0-9

- Setup:
  - Get a large collection of example images, each labeled with a digit
  - Note: someone has to hand label all this data!
  - Want to learn to predict labels of new, future digit images

- Features: The attributes used to make the digit decision
  - Pixels: (6,8)=ON
  - Shape Patterns: NumComponents, AspectRatio, NumLoops
  - …
  - Features are increasingly induced rather than crafted


0


1

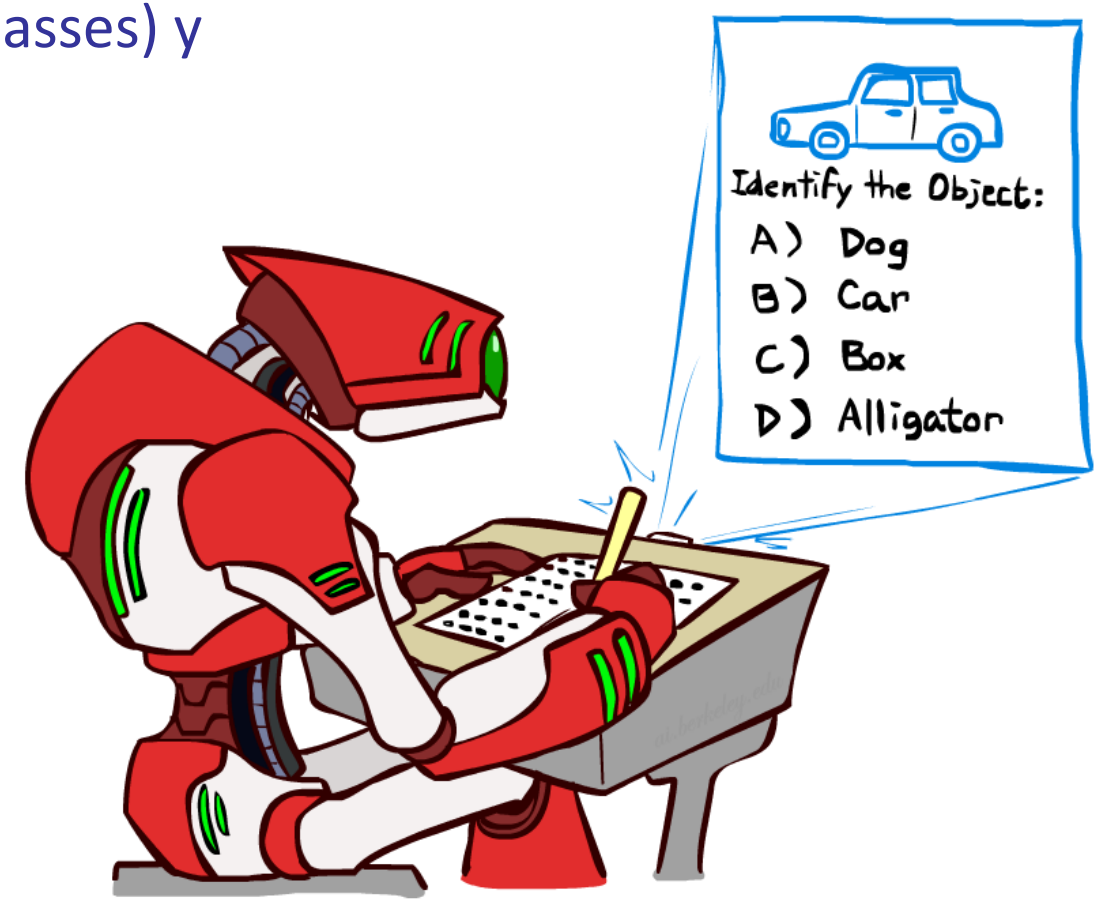

2


1


??

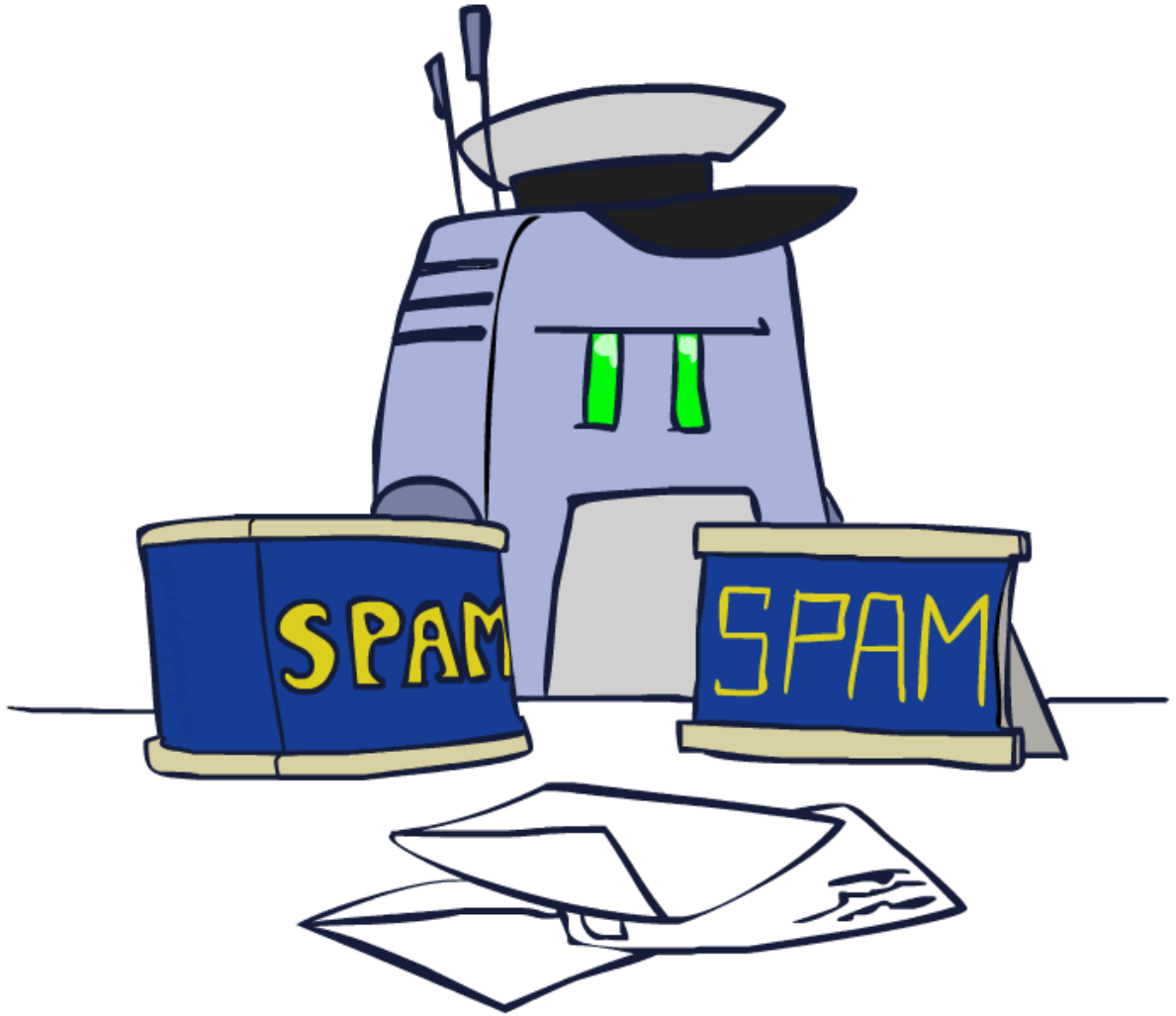
Other Classification Tasks

- Classification: given inputs x, predict labels (classes) y
  - Binary classification (2 classes)
  - Multiclass classification (>2 classes)
- Examples:
  - Medical diagnosis (input: symptoms, classes: diseases)
  - Fraud detection (input: account activity, classes: fraud / no fraud)
  - Automatic essay grading (input: document, classes: grades)
  - Customer service email routing
  - Review sentiment
  - Language ID
  - … many more



- Classification is an important commercial technology!

Model-Based Classification

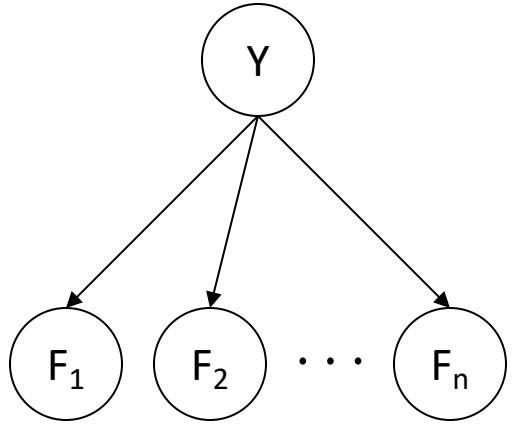


Model-Based Classification

- Model-based approach
  - Build a model (e.g. Bayes' net) where both the output label and input features are random variables
  - Instantiate any observed features
  - Query for the distribution of the label conditioned on the features
- Challenges
  - What structure should the BN have?
  - How should we learn its parameters?

Naïve Bayes for Digits

- Naïve Bayes: Assume all features are independent effects of the label



- Simple digit recognition version:
  - One feature (variable) F_{ij} for each grid position <i,j>
  - Feature values are on / off, based on whether intensity is more or less than 0.5 in underlying image
  - Each input maps to a feature vector, e.g.

$$\rightarrow \langle F_{0,0} = 0 \;\; F_{0,1} = 0 \;\; F_{0,2} = 1 \;\; F_{0,3} = 1 \;\; F_{0,4} = 0 \;\; \ldots F_{15,15} = 0 \rangle$$

  - Here: lots of features, each is binary valued

- Naïve Bayes model: $P(Y|F_{0,0} \ldots F_{15,15}) \propto P(Y) \prod_{i,j} P(F_{i,j}|Y)$

- What do we need to learn?

General Naïve Bayes

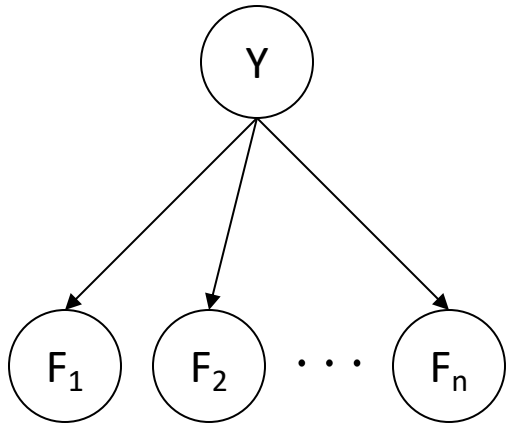
- A general Naive Bayes model:

|Y| parameters

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

|Y| x |F|^n values

n x |F| x |Y| parameters



- We only have to specify how each feature depends on the class
- Total number of parameters is *linear* in n
- Model is very simplistic, but often works anyway

Inference for Naïve Bayes

- Goal: compute posterior distribution over label variable Y
  - Step 1: get joint probability of label and evidence for each label

$$P(Y, f_1 \dots f_n) = \begin{bmatrix} P(y_1, f_1 \dots f_n) \\ P(y_2, f_1 \dots f_n) \\ \vdots \\ P(y_k, f_1 \dots f_n) \end{bmatrix} \Rightarrow \begin{bmatrix} P(y_1) \prod_i P(f_i|y_1) \\ P(y_2) \prod_i P(f_i|y_2) \\ \vdots \\ P(y_k) \prod_i P(f_i|y_k) \end{bmatrix}$$

$$\Rightarrow \frac{\begin{bmatrix} P(y_1) \prod_i P(f_i|y_1) \\ P(y_2) \prod_i P(f_i|y_2) \\ \vdots \\ P(y_k) \prod_i P(f_i|y_k) \end{bmatrix}}{P(f_1 \dots f_n)} \Rightarrow P(Y|f_1 \dots f_n)$$

  - Step 2: sum to get probability of evidence
  - Step 3: normalize by dividing Step 1 by Step 2

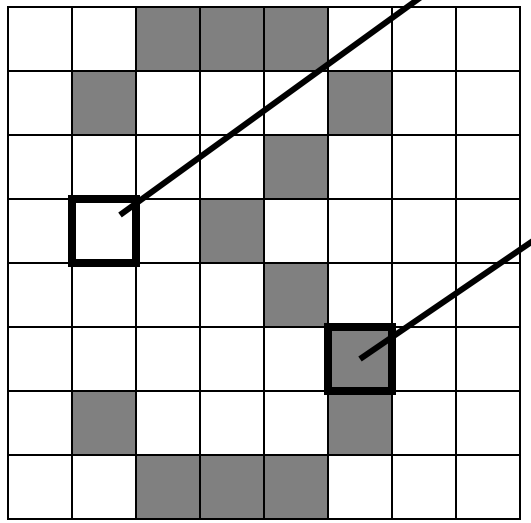
General Naïve Bayes

- What do we need in order to use Naïve Bayes?
  - Inference method (we just saw this part)
    - Start with a bunch of probabilities: P(Y) and the $P(F_i|Y)$ tables
    - Use standard inference to compute $P(Y|F_1 \ldots F_n)$
    - Nothing new here
  - Estimates of local conditional probability tables
    - P(Y), the prior over labels
    - $P(F_i|Y)$ for each feature (evidence variable)
    - These probabilities are collectively called the *parameters* of the model and denoted by θ
    - Up until now, we assumed these appeared by magic, but…
    - …they typically come from training data counts: we'll look at this soon

Example: Conditional Probabilities

$P(Y)$

1	0.1
2	0.1
3	0.1
4	0.1
5	0.1
6	0.1
7	0.1
8	0.1
9	0.1
0	0.1



$P(F_{3,1} = on|Y)$

1	0.01
2	0.05
3	0.05
4	0.30
5	0.80
6	0.90
7	0.05
8	0.60
9	0.50
0	0.80

$P(F_{5,5} = on|Y)$

1	0.05
2	0.01
3	0.90
4	0.80
5	0.90
6	0.90
7	0.25
8	0.85
9	0.60
0	0.80

Naïve Bayes for Text

- Bag-of-words Naïve Bayes:
  - Features: W_i is the word at position i
  - As before: predict label conditioned on feature variables (spam vs. ham)
  - As before: assume features are conditionally independent given label
  - New: each W_i is identically distributed
- Generative model: $P(Y, W_1 \dots W_n) = P(Y) \prod_i P(W_i|Y)$

Word at position i, not i^{th} word in the dictionary!

- "Tied" distributions and bag-of-words
  - Usually, each variable gets its own conditional probability distribution P(F|Y)
  - In a bag-of-words model
    - Each position is identically distributed
    - All positions share the same conditional probs P(W|Y)
    - Why make this assumption?
  - Called "bag-of-words" because model is insensitive to word order or reordering

Example: Spam Filtering

- Model: $P(Y, W_1 \dots W_n) = P(Y) \prod_i P(W_i|Y)$
- What are the parameters?

$P(Y)$

ham	0.66
spam	0.33

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

the	0.0156
to	0.0153
and	0.0115
of	0.0095
you	0.0093
a	0.0086
with	0.0080
from	0.0075
...	

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

the	0.0210
to	0.0133
of	0.0119
2002	0.0110
with	0.0108
from	0.0107
and	0.0105
a	0.0100
...	

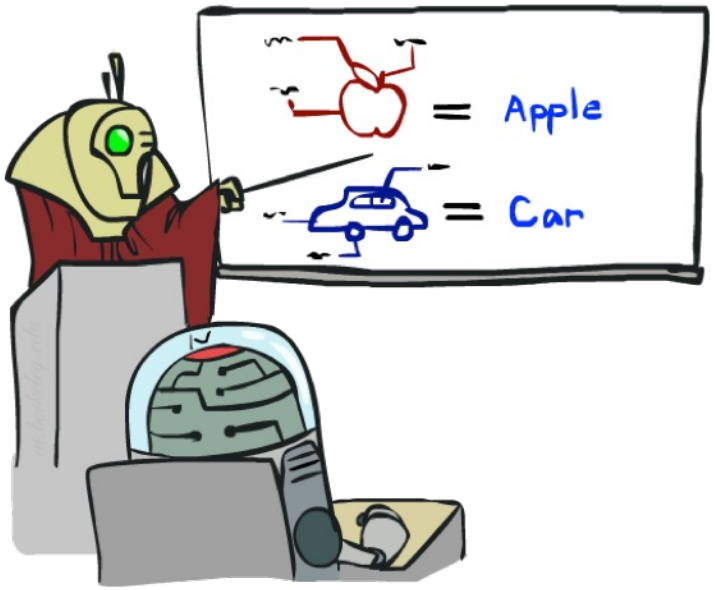
- Where do these tables come from?

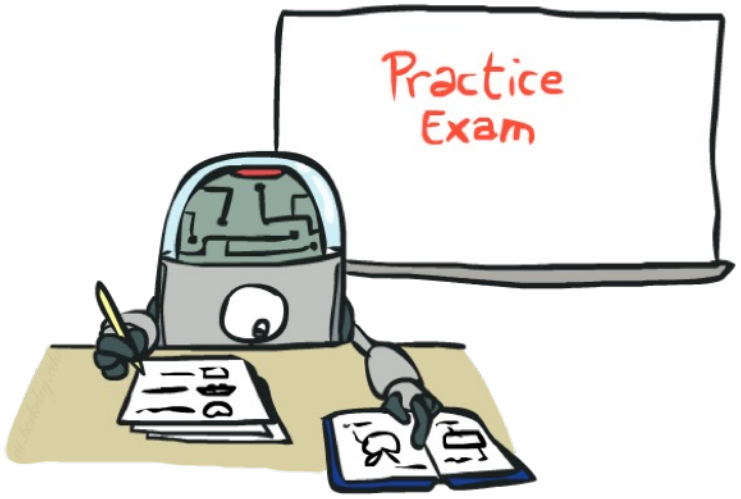
Spam Example

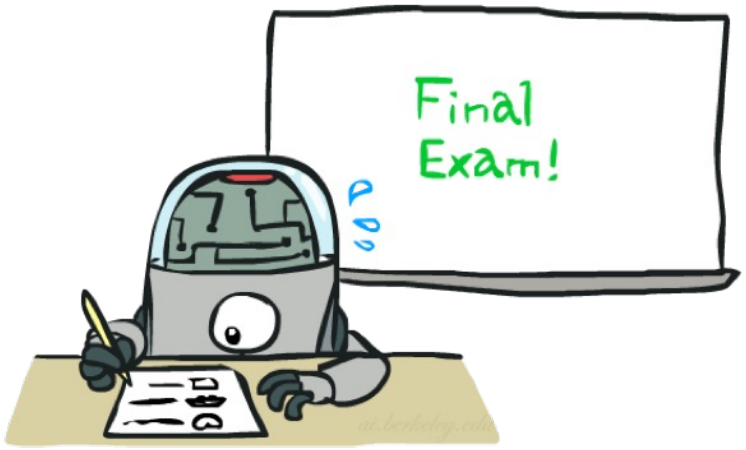
Word	P(w|spam)	P(w|ham)	Tot Spam	Tot Ham
(prior)	0.33333	0.66666	-1.1	-0.4

P(spam | w) = 98.9

Training and Testing







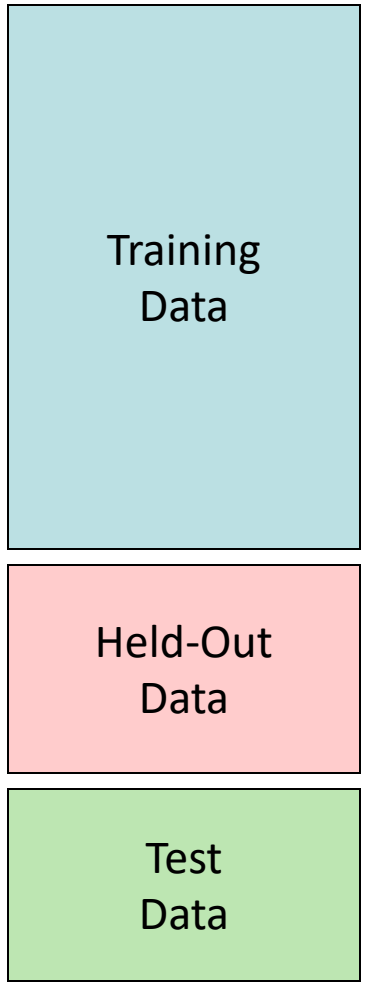
Empirical Risk Minimization

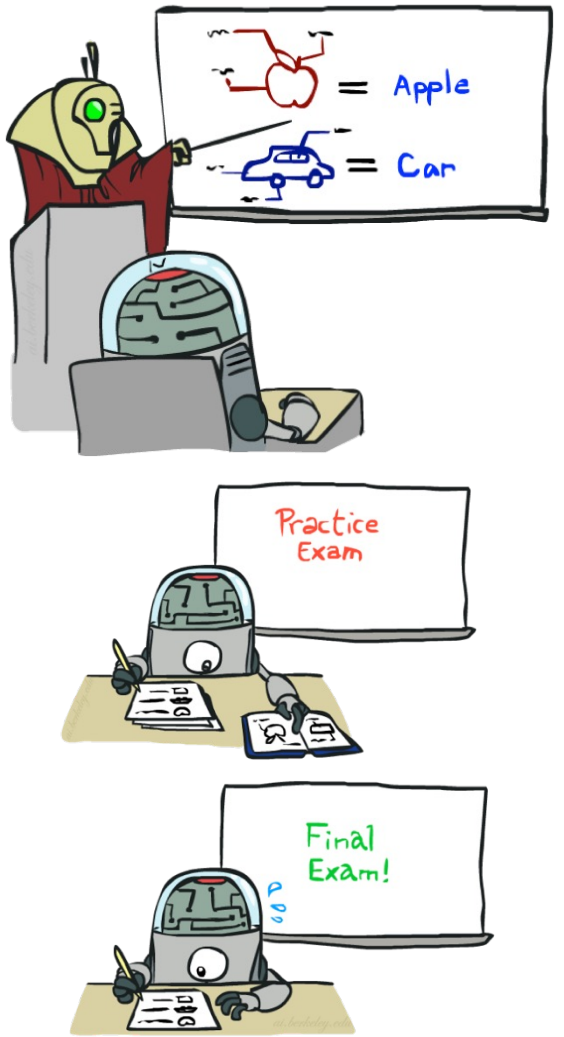
- Empirical risk minimization
  - Basic principle of machine learning
  - We want the model (classifier, etc) that does best on the true test distribution
  - Don’t know the true distribution so pick the best model on our actual training set
  - Finding “the best” model on the training set is phrased as an optimization problem

- Main worry: overfitting to the training set
  - Better with more training data (less sampling variance, training more like test)
  - Better if we limit the complexity of our hypotheses (regularization and/or small hypothesis spaces)

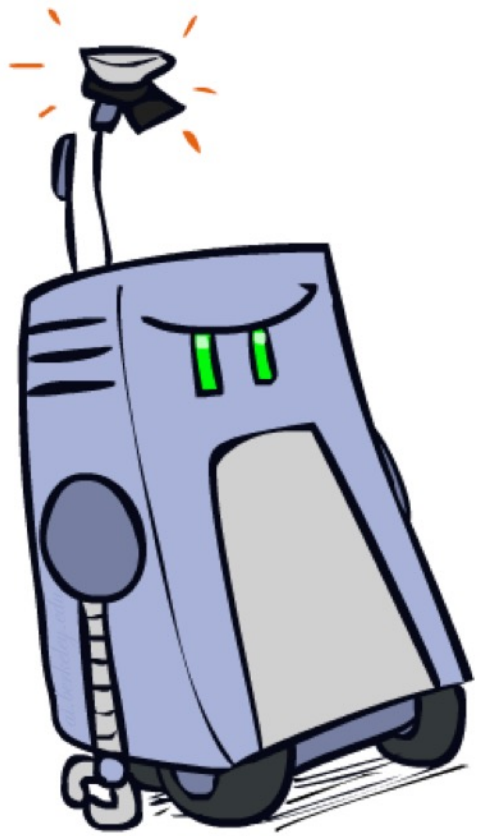
Important Concepts

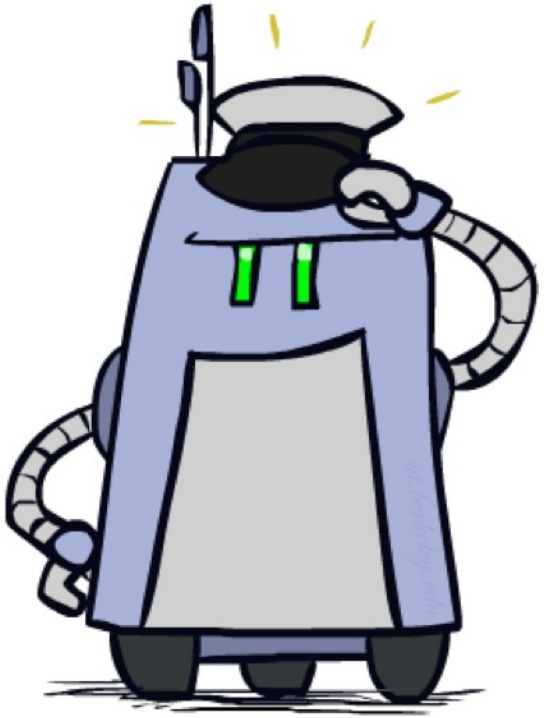
- Data: labeled instances (e.g. emails marked spam/ham)
  - Training set
  - Held out set ("development" or "validation" set)
  - Test set
- Features: attribute-value pairs which characterize each x
- Experimentation cycle
  - Learn parameters (e.g. model probabilities) on training set
  - (Tune hyperparameters on held-out set)
  - Compute accuracy of test set
  - Very important: never "peek" at the test set!
- Evaluation (many metrics possible, e.g. accuracy)
  - Accuracy: fraction of instances predicted correctly
- Overfitting and generalization
  - Want a classifier which does well on *test* data
  - Overfitting: fitting the training data very closely, but not generalizing well
  - We'll investigate overfitting and generalization formally in a few lectures



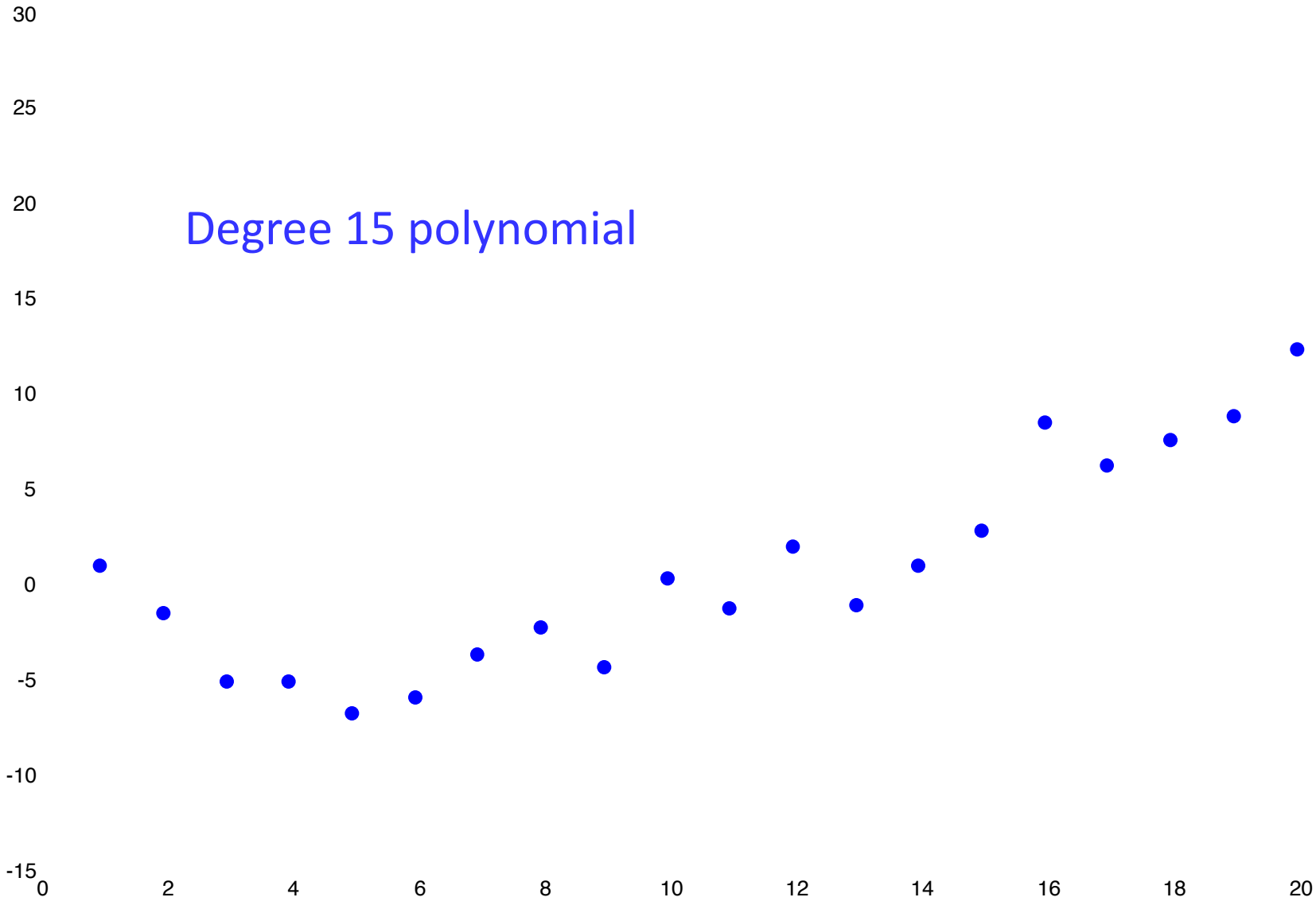


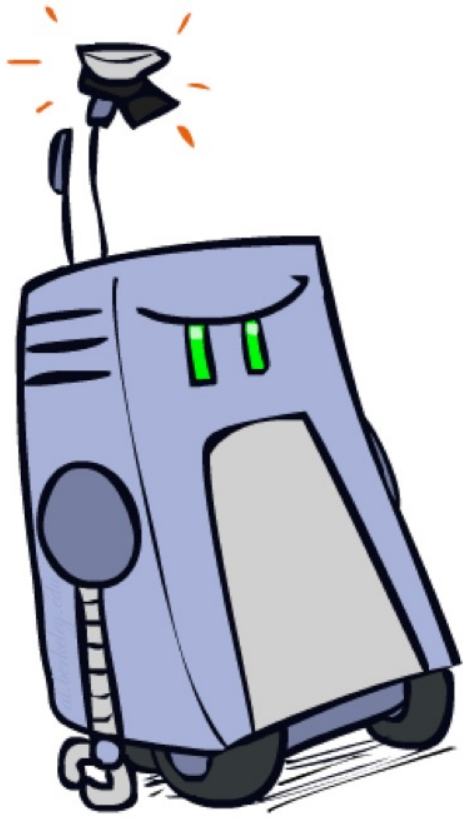
Generalization and Overfitting





Overfitting





Example: Overfitting

$P(\text{features}, C = 2)$

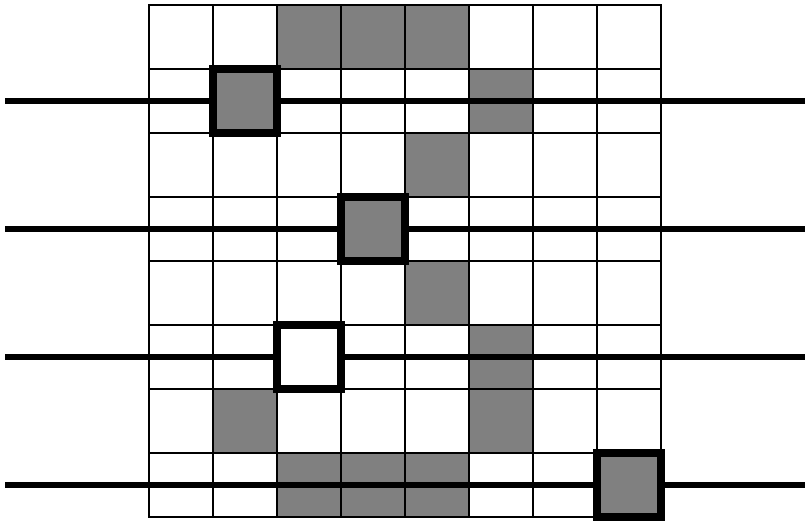
$P(C = 2) = 0.1$

$P(\text{on}|C = 2) = 0.8$

$P(\text{on}|C = 2) = 0.1$

$P(\text{off}|C = 2) = 0.1$

$P(\text{on}|C = 2) = 0.01$



$P(\text{features}, C = 3)$

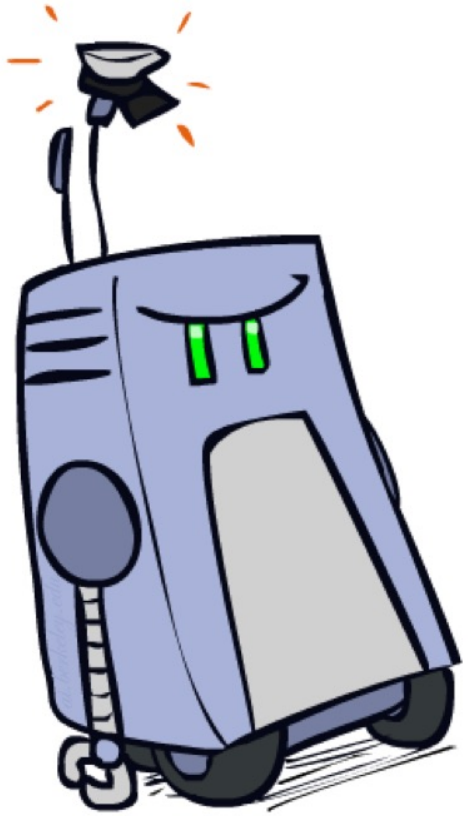
$P(C = 3) = 0.1$

$P(\text{on}|C = 3) = 0.8$

$P(\text{on}|C = 3) = 0.9$

$P(\text{off}|C = 3) = 0.7$

$P(\text{on}|C = 3) = 0.0$



2 wins!!

Example: Overfitting

- Posteriors determined by *relative* probabilities (odds ratios):

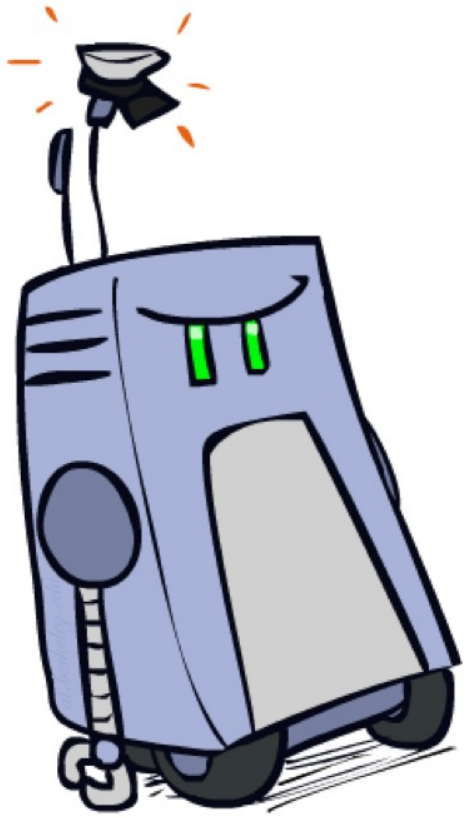
$$\frac{P(W|\text{ham})}{P(W|\text{spam})}$$

```
south-west : inf
nation     : inf
morally    : inf
nicely     : inf
extent     : inf
seriously  : inf
...
```

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

```
screens    : inf
minute     : inf
guaranteed : inf
$205.00    : inf
delivery   : inf
signature  : inf
...
```

What went wrong here?



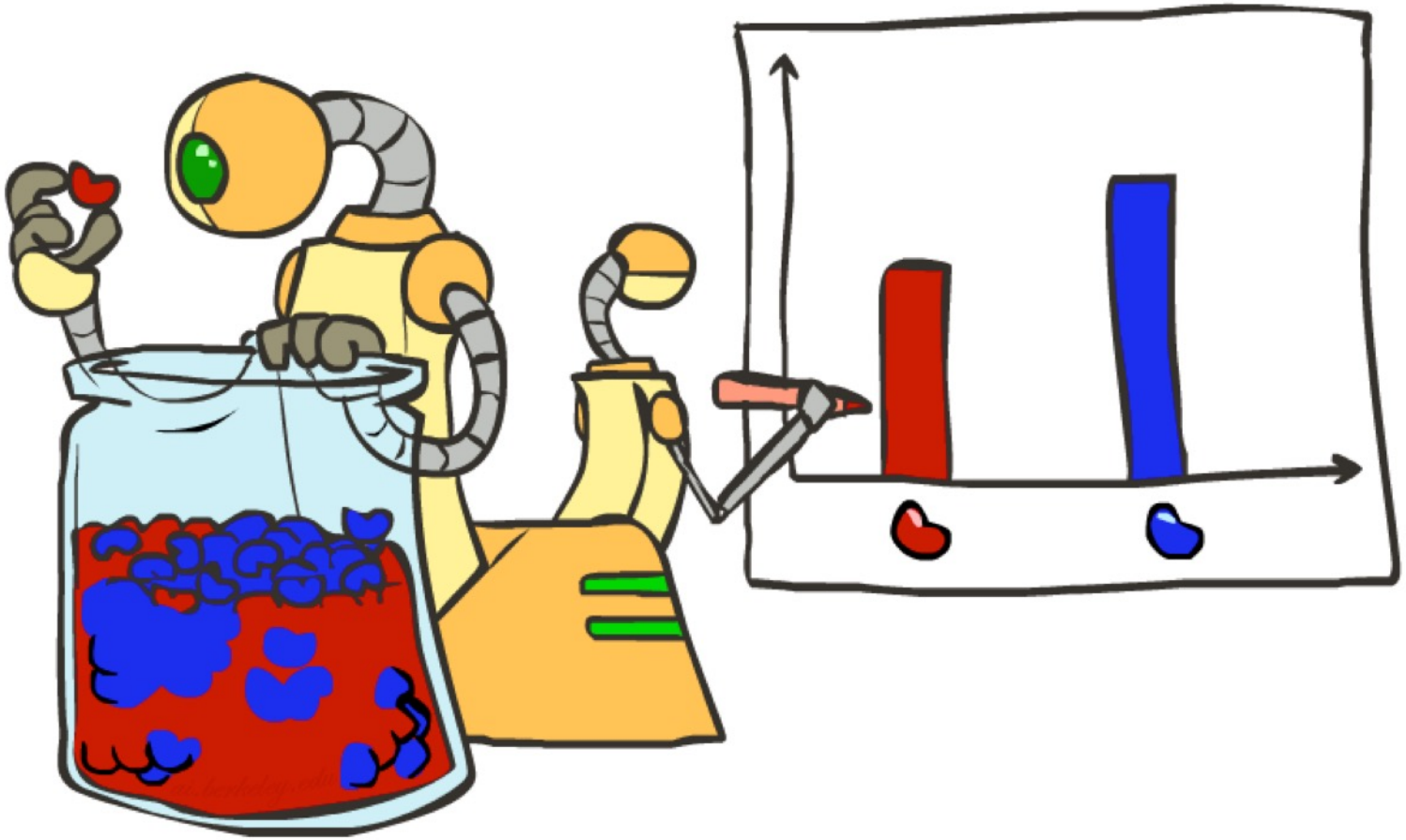
Generalization and Overfitting

- Relative frequency parameters will overfit the training data!
  - Just because we never saw a 3 with pixel (15,15) on during training doesn't mean we won't see it at test time
  - Unlikely that every occurrence of "minute" is 100% spam
  - Unlikely that every occurrence of "seriously" is 100% ham
  - What about all the words that don't occur in the training set at all?
  - In general, we can't go around giving unseen events zero probability

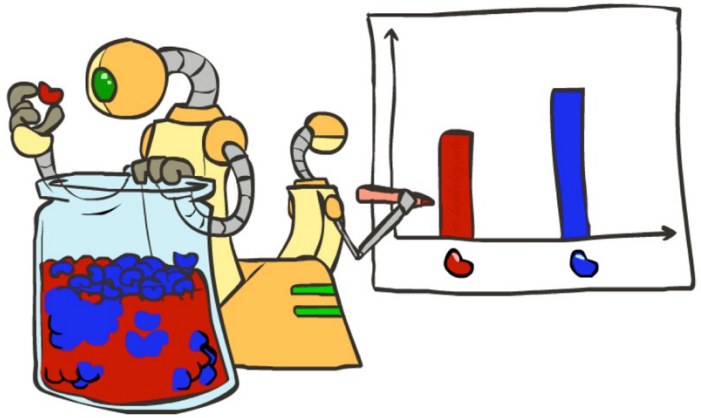
- As an extreme case, imagine using the entire email as the only feature (e.g. document ID)
  - Would get the training data perfect (if deterministic labeling)
  - Wouldn't *generalize* at all
  - Just making the bag-of-words assumption gives us some generalization, but isn't enough

- To generalize better: we need to smooth or regularize the estimates

Parameter Estimation



Parameter Estimation



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

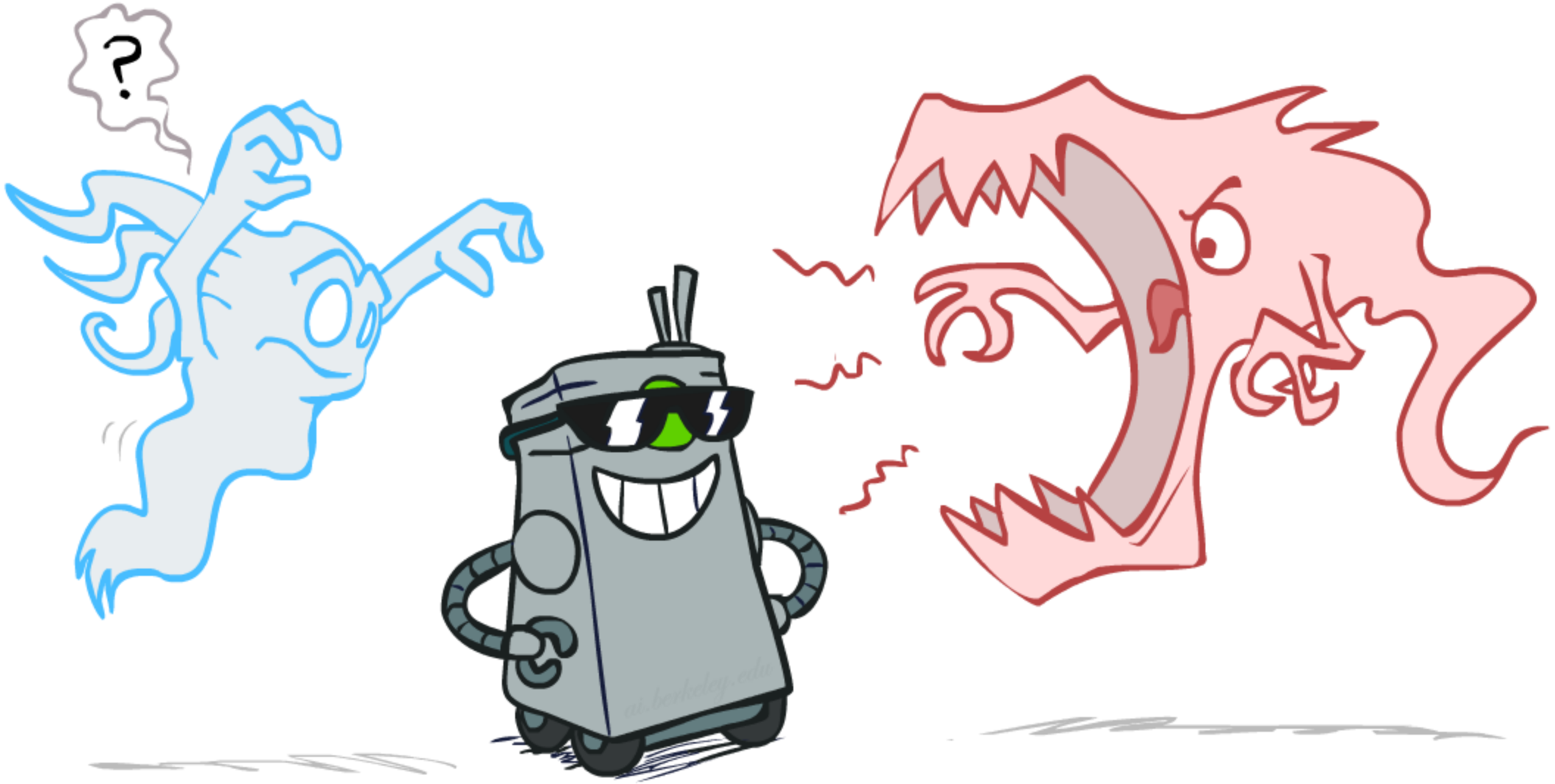
$$P_{\text{ML}}(x) = \frac{\text{count}(x)}{\text{total samples}}$$

$$P_{\text{ML}}(\text{r}) = 2/3$$

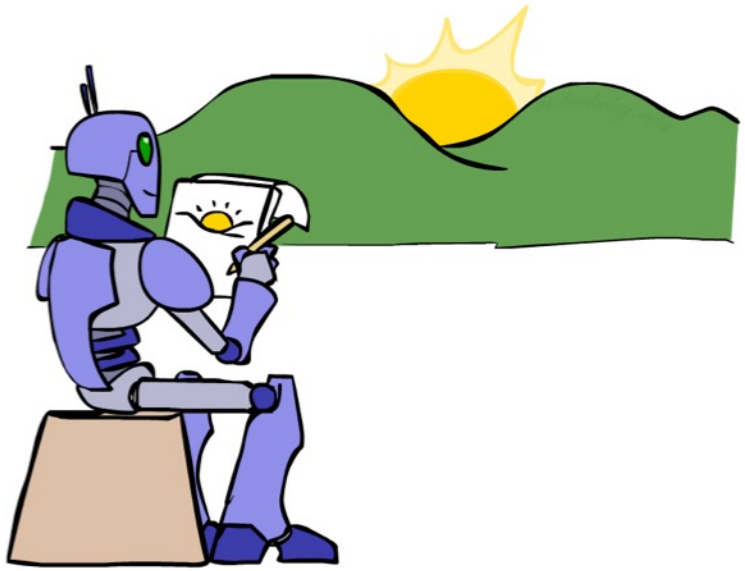
  - This is the estimate that maximizes the *likelihood of the data*

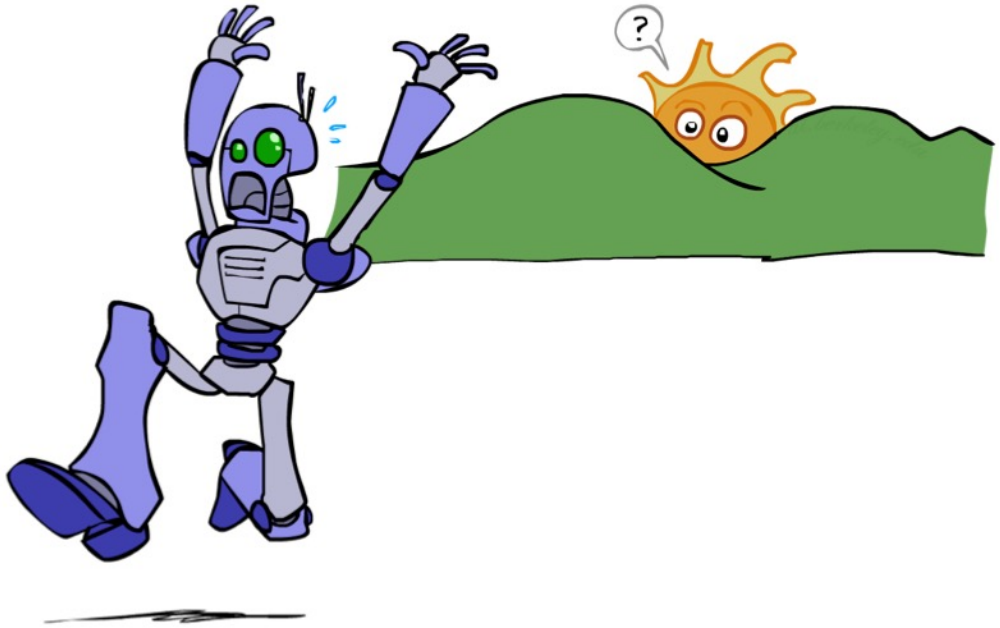
$$L(x, \theta) = \prod_i P_\theta(x_i)$$

Smoothing



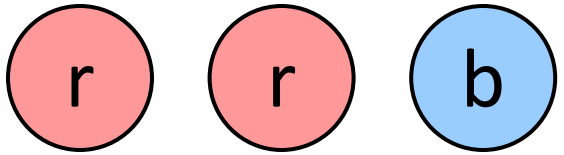
Unseen Events





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

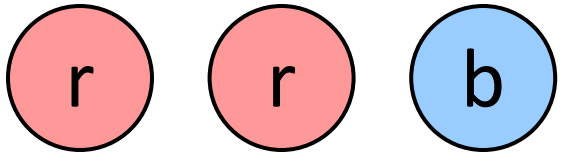
- Laplace's estimate (extended)– "Add-k smoothing":
  - Pretend you saw every outcome k extra times

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

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

- Laplace for conditionals:
  - Smooth each condition independently:

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



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

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

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

[Bonus] Estimation: 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)

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

  - What if α is 0? 1?
- For even better ways to estimate parameters, as well as details of the math, see cs281a, cs288

Real NB: Smoothing

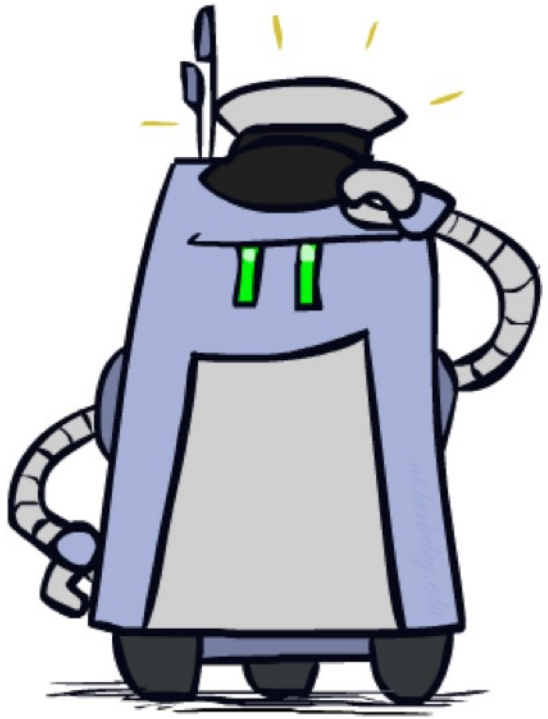
- For real classification problems, smoothing is critical
- New odds ratios:

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

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

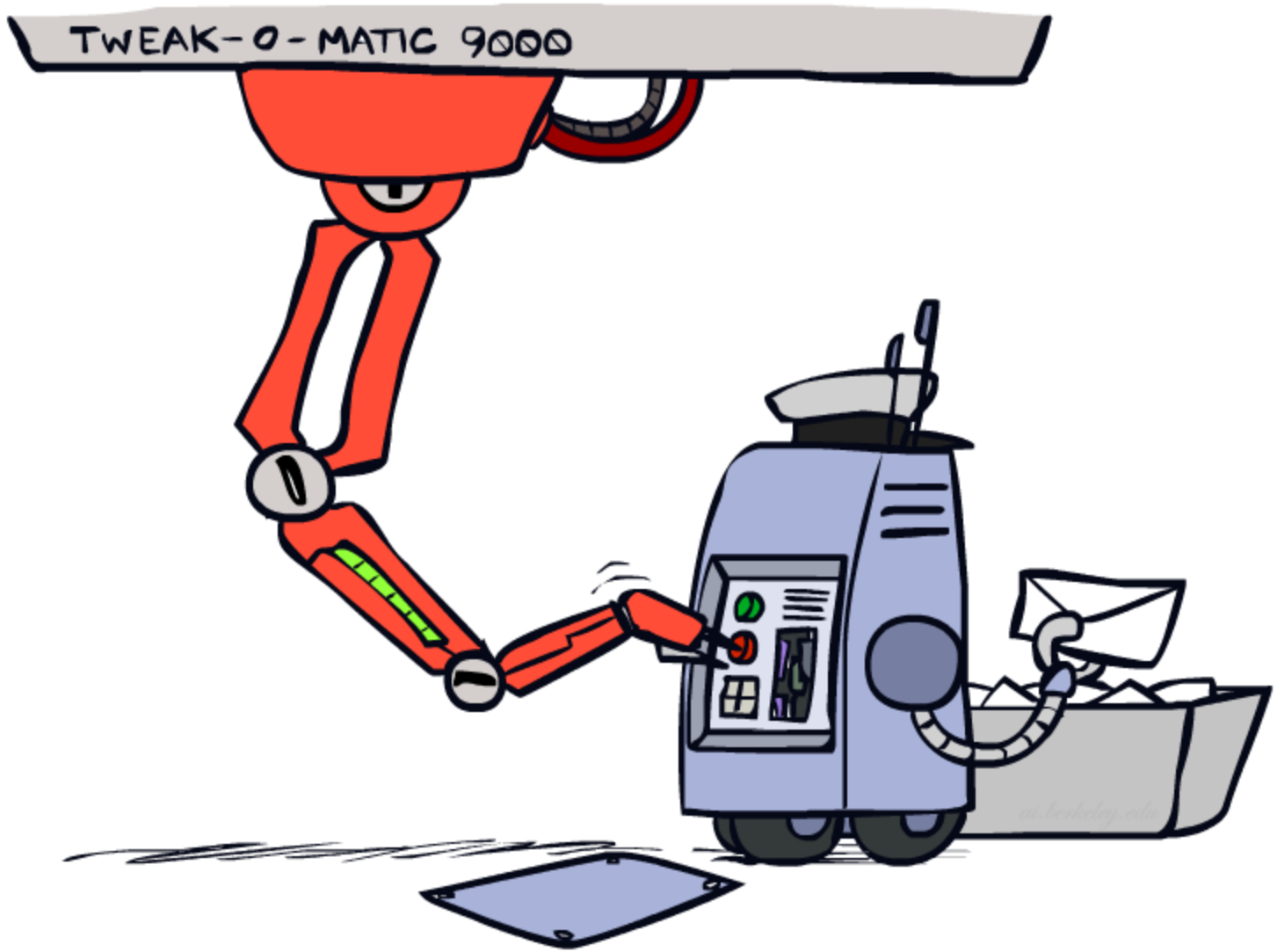
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

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



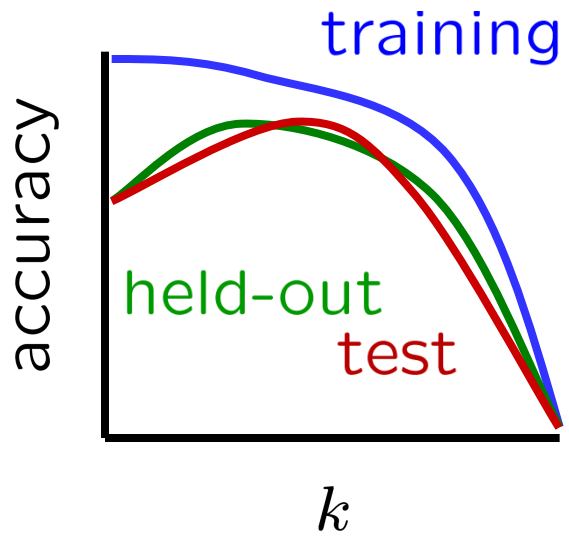
Do these make more sense?

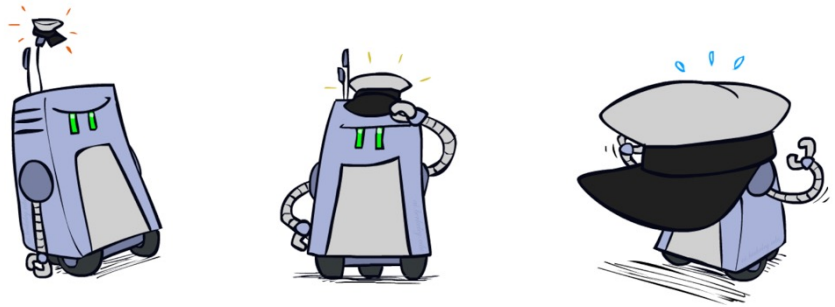
Tuning



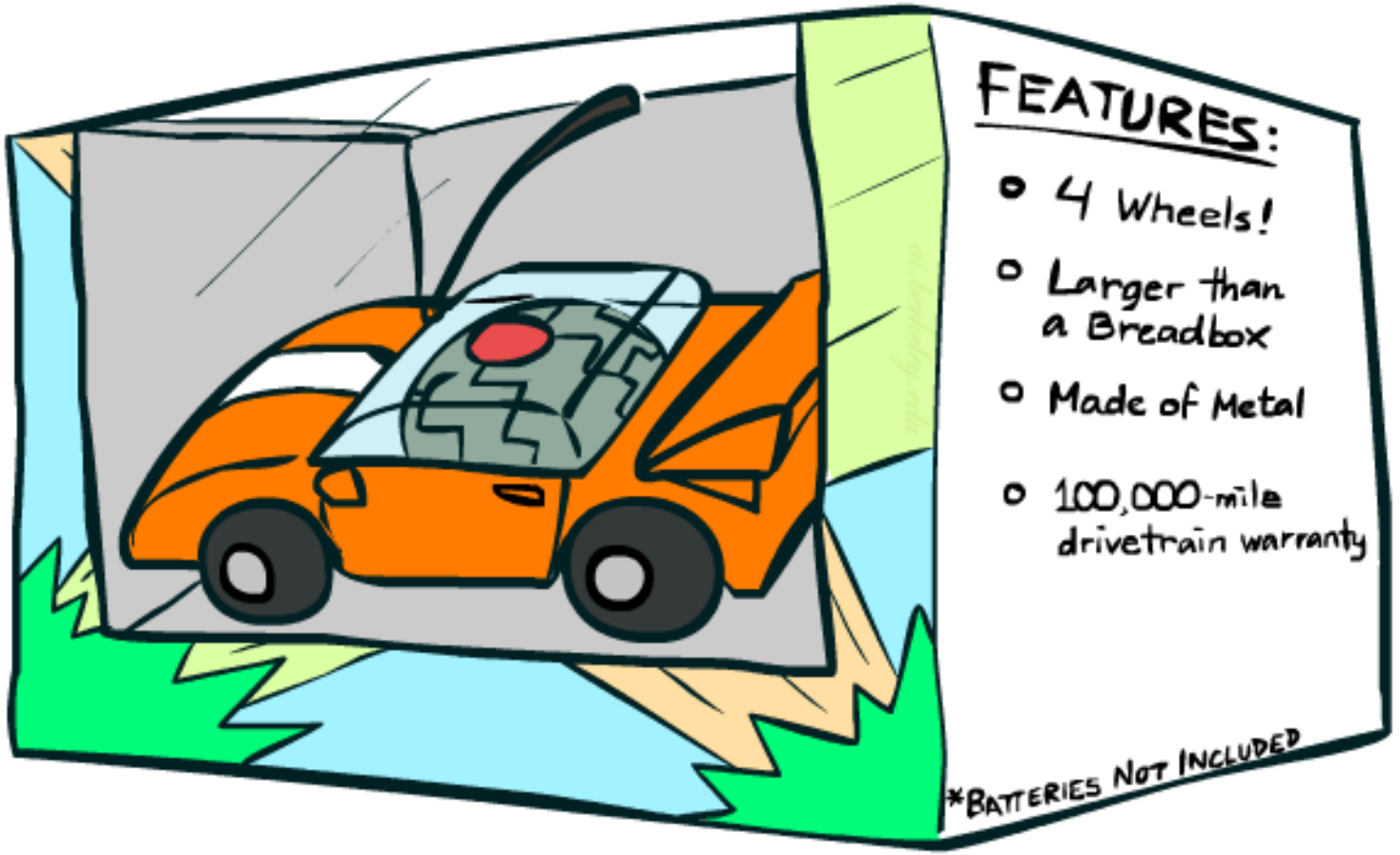
Tuning on Held-Out Data

- 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





Features


FEATURES:
4 Wheels!
Larger than a Breadbox
Made of Metal
100,000-mile drivetrain warranty
*Batteries Not Included

Errors, and What to Do

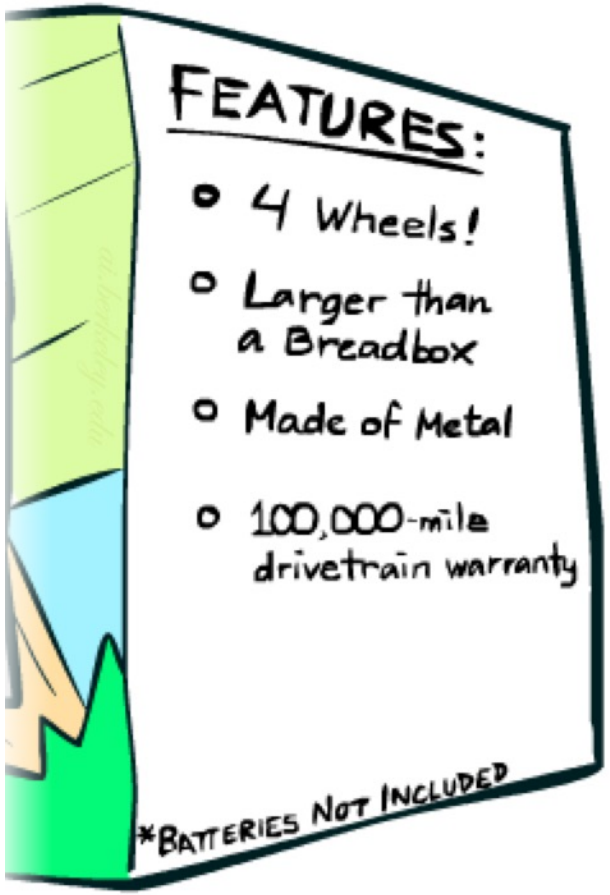
- Examples of errors

> Dear GlobalSCAPE Customer,
>
> GlobalSCAPE has partnered with ScanSoft to offer you the latest version of OmniPage Pro, for just $99.99* - the regular list price is $499! The most common question we've received about this offer is - Is this genuine? We would like to assure you that this offer is authorized by ScanSoft, is genuine and valid. You can get the . . .

> . . . To receive your $30 Amazon.com promotional certificate, click through to
>
> http://www.amazon.com/apparel
>
> and see the prominent link for the $30 offer. All details are there. We hope you enjoyed receiving this message. However, if you'd rather not receive future e-mails announcing new store launches, please click . . .

What to Do About Errors?

- Need more features– words aren't enough!
  - Have you emailed the sender before?
  - Have 1K other people just gotten the same email?
  - Is the sending information consistent?
  - Is the email in ALL CAPS?
  - Do inline URLs point where they say they point?
  - Does the email address you by (your) name?
- Can add these information sources as new variables in the NB model
- Later this week we'll talk about classifiers which let you easily add arbitrary features more easily, and, later, how to induce new features



Baselines

- First step: get a baseline
  - Baselines are very simple “straw man” procedures
  - Help determine how hard the task is
  - Help know what a “good” accuracy is

- Weak baseline: most frequent label classifier
  - Gives all test instances whatever label was most common in the training set
  - E.g. for spam filtering, might label everything as ham
  - Accuracy might be very high if the problem is skewed
  - E.g. calling everything “ham” gets 66%, so a classifier that gets 70% isn’t very good…

- For real research, usually use previous work as a (strong) baseline

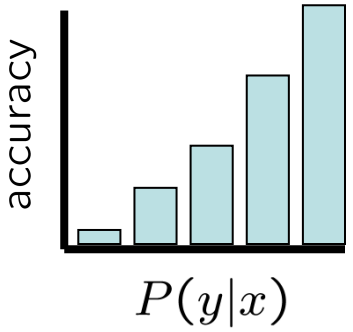
Confidences from a Classifier

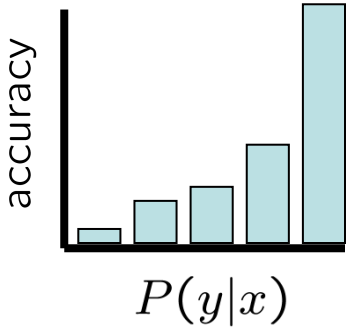
- The confidence of a probabilistic classifier:
  - Posterior probability of the top label

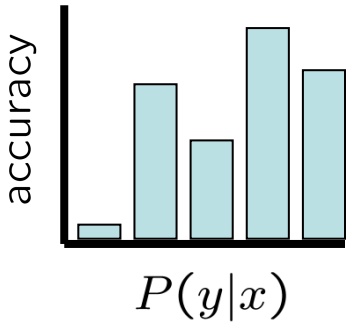
$$\text{confidence}(x) = \max_y P(y|x)$$

  - 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

CS 188: Artificial Intelligence

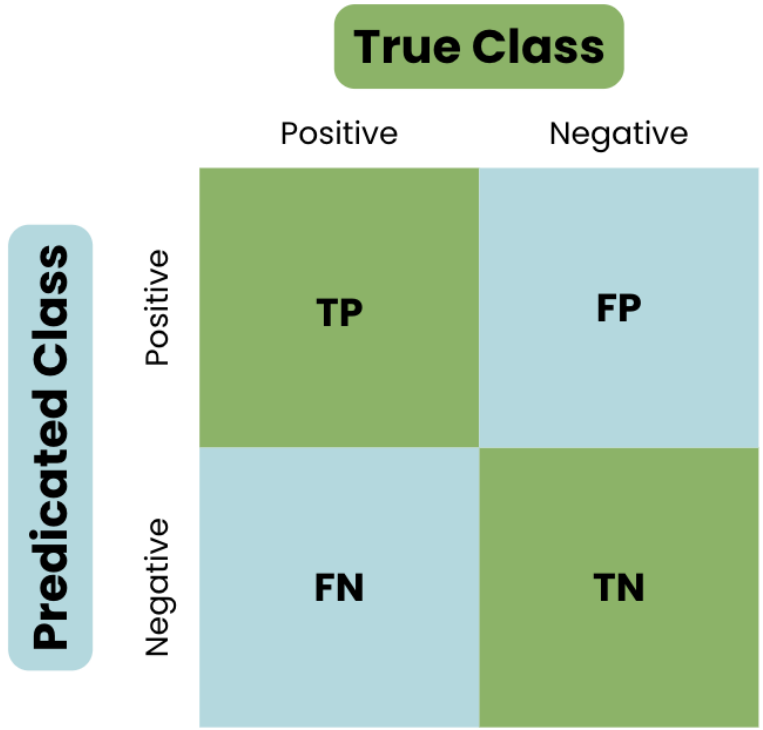
Machine Learning

Summer 2024: Eve Fleisig & Evgeny Pobachienko

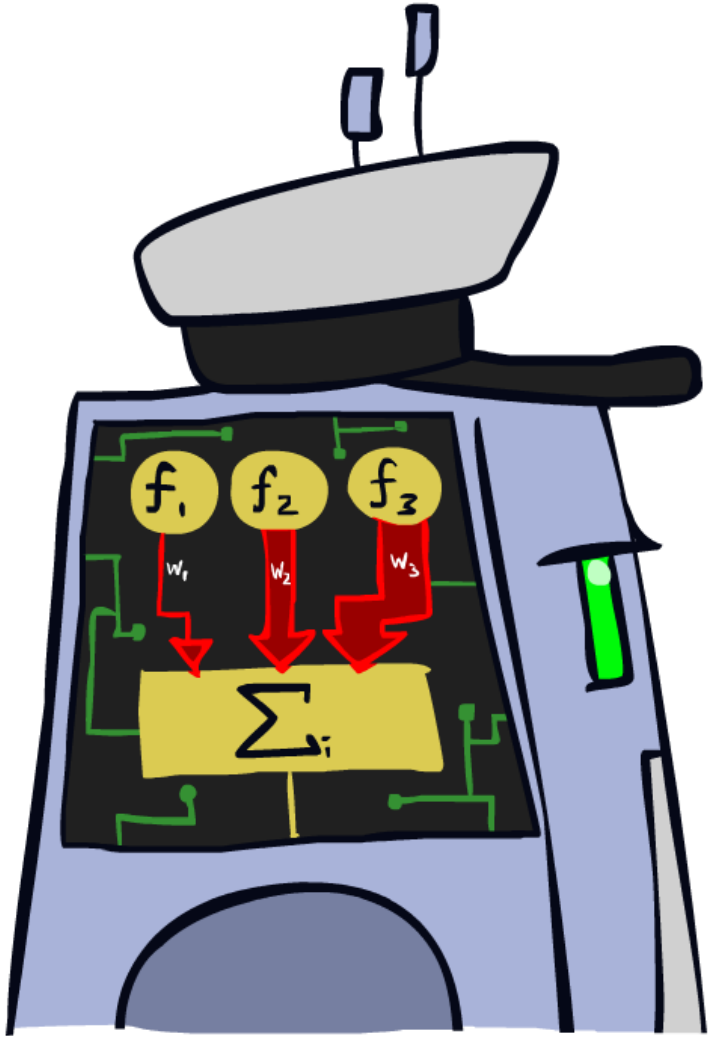
[Slides based on those by Nicholas Tomlin, Dan Klein and Pieter Abbeel for CS188 Intro to AI at UC Berkeley. CS188 materials are available at http://ai.berkeley.edu.]

Demo: Catching AI-Generated Text

- Feature design
  - Complexity in feature design vs. model design
- Evaluation
  - Accuracy, precision & recall, F1 score
- Generalization
- Calibration
- Robustness



Linear Classifiers



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
...
```

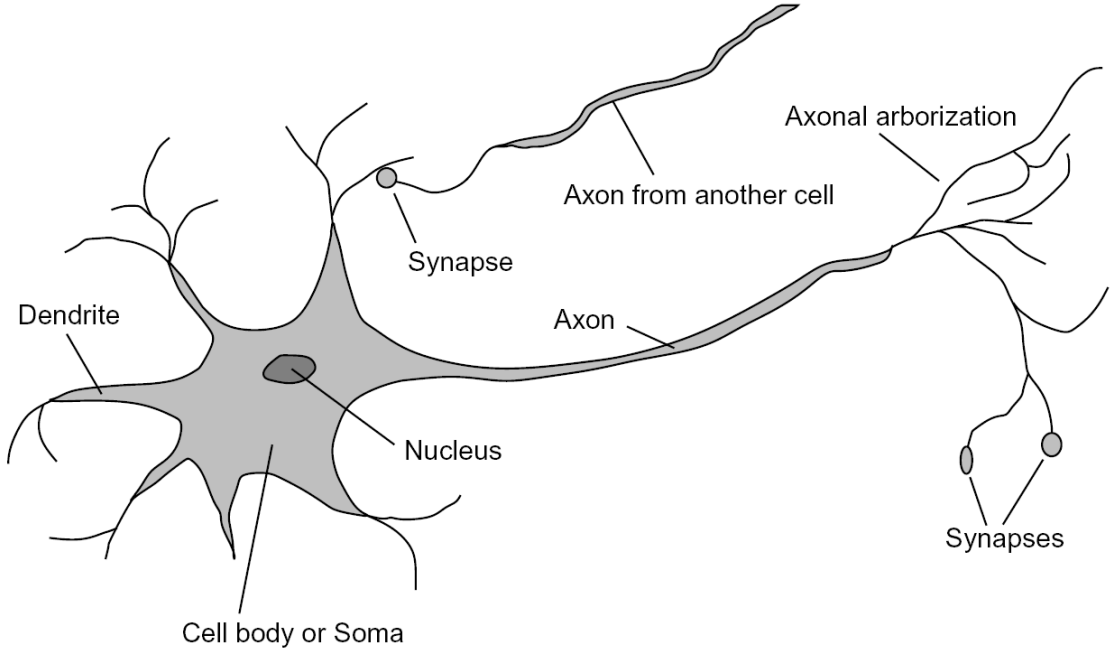
```
PIXEL-7,12   : 1
PIXEL-7,13   : 0
...
NUM_LOOPS    : 1
...
```

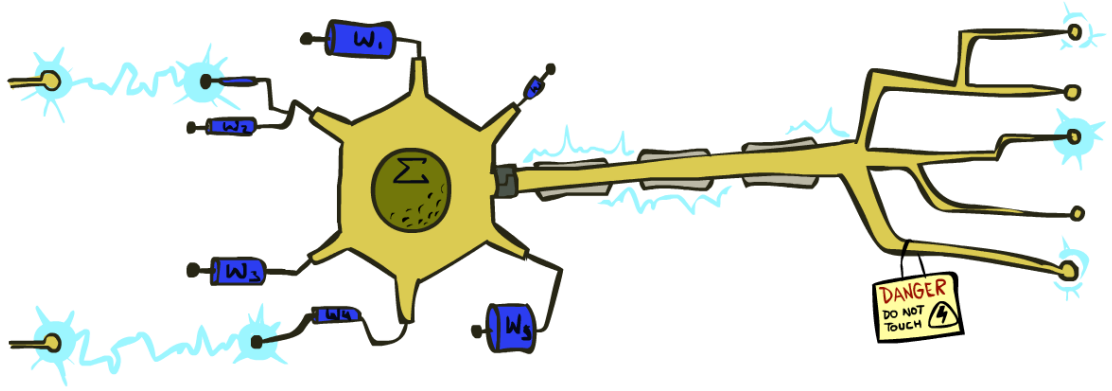
SPAM
or
+

“2”

Some (Simplified) Biology

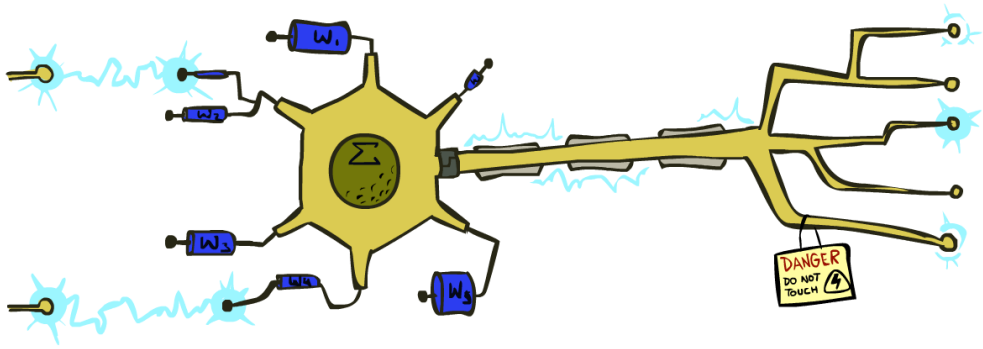
- Very loose inspiration: human neurons





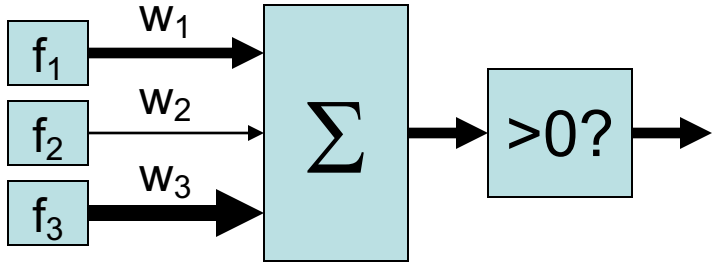
Linear Classifiers

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



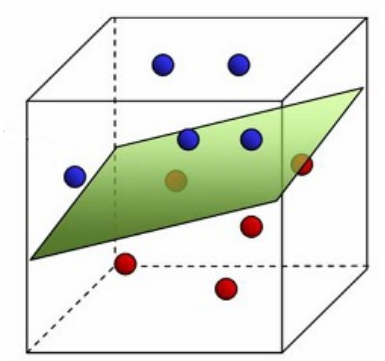
$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

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

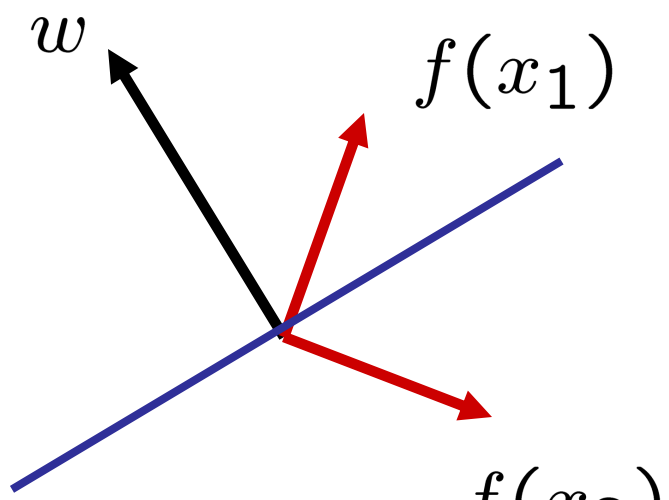


Weights

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



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

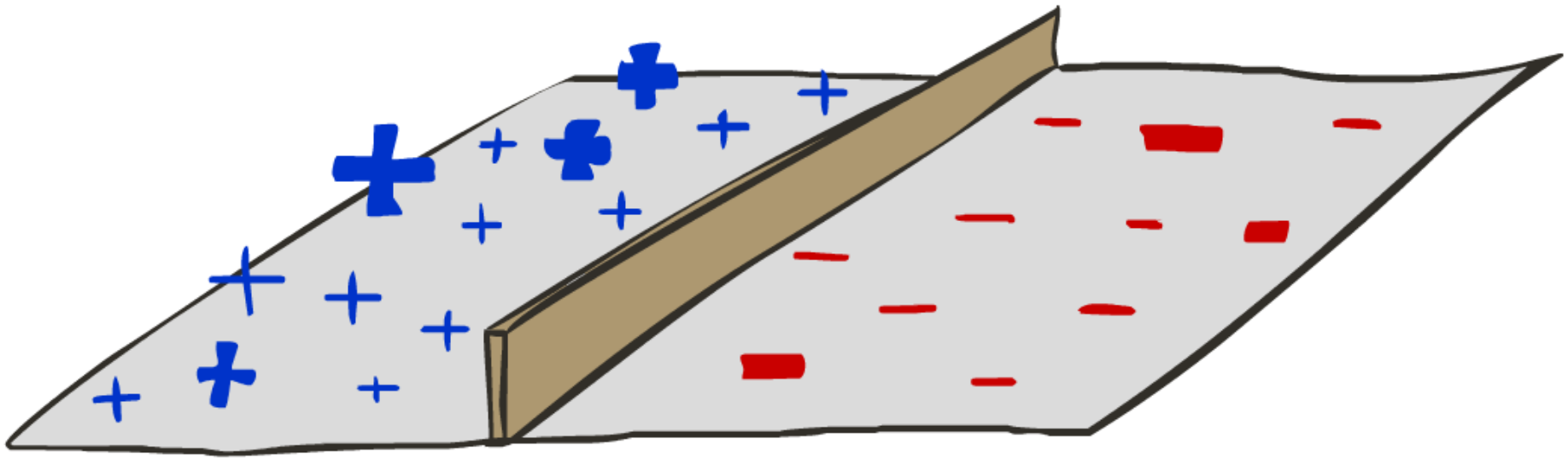



```
# free       : 2
YOUR_NAME    : 0
MISSPELLED   : 2
FROM_FRIEND  : 0
...
```

```
# free       : 0
YOUR_NAME    : 1
MISSPELLED   : 1
FROM_FRIEND  : 1
...
```

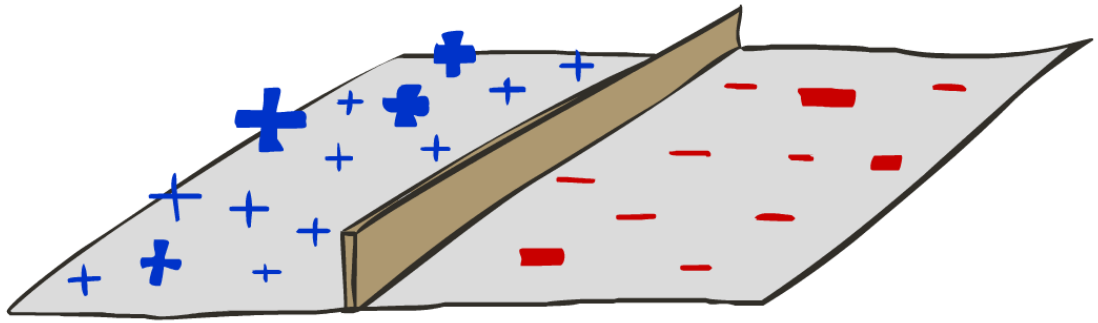
Dot product $w \cdot f$ positive means the positive class

Decision Rules



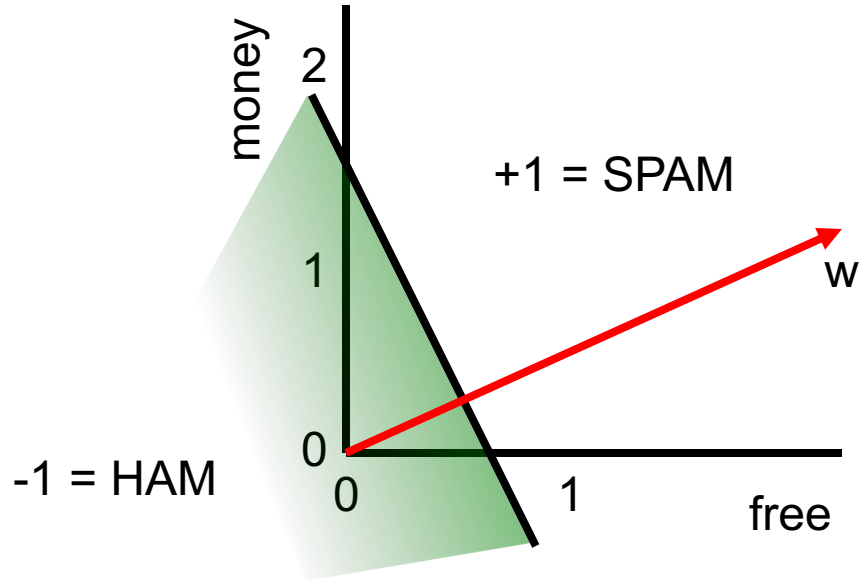
Binary Decision Rule

- 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
...
```

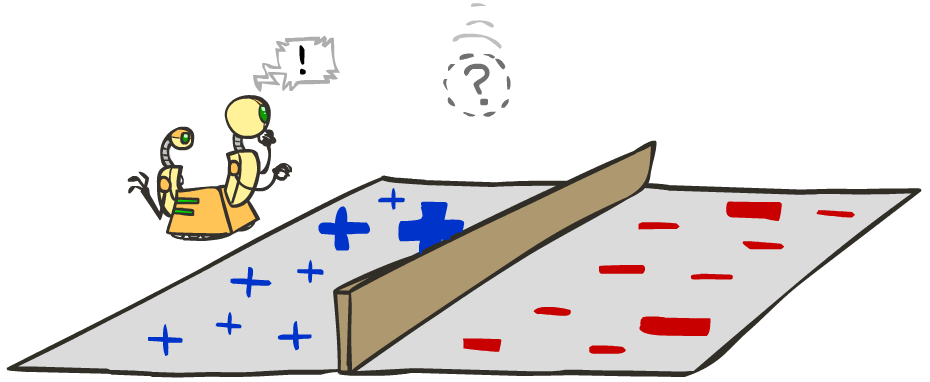


$f \cdot w = 0$

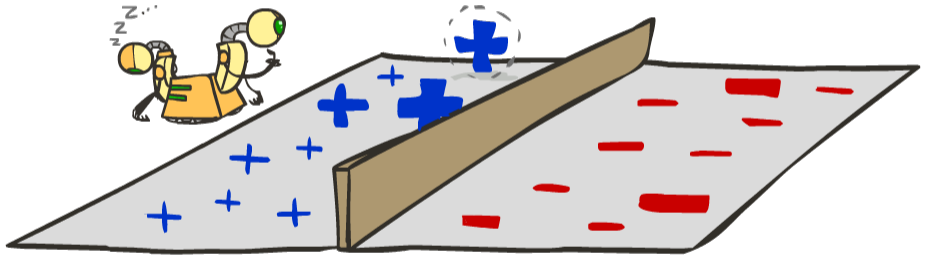
Weight Updates

Learning: Binary Perceptron

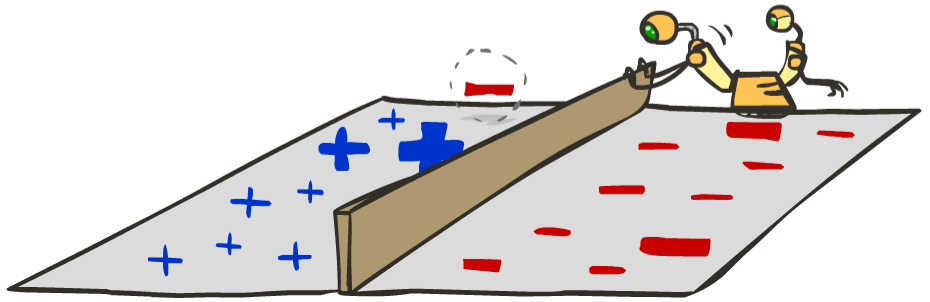
- Start with weights = 0
- For each training instance:
  - Classify with current weights



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



  - If wrong: adjust the weight vector



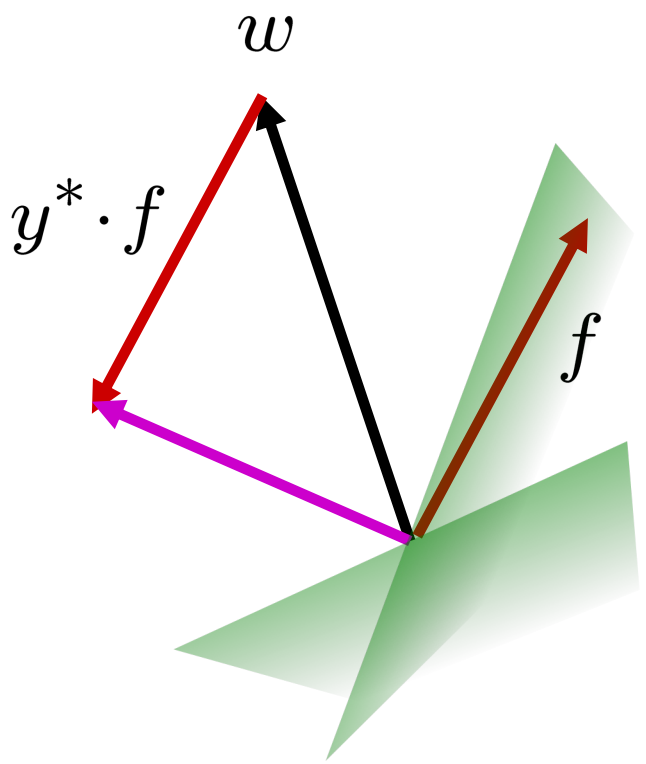
Learning: Binary Perceptron

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

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

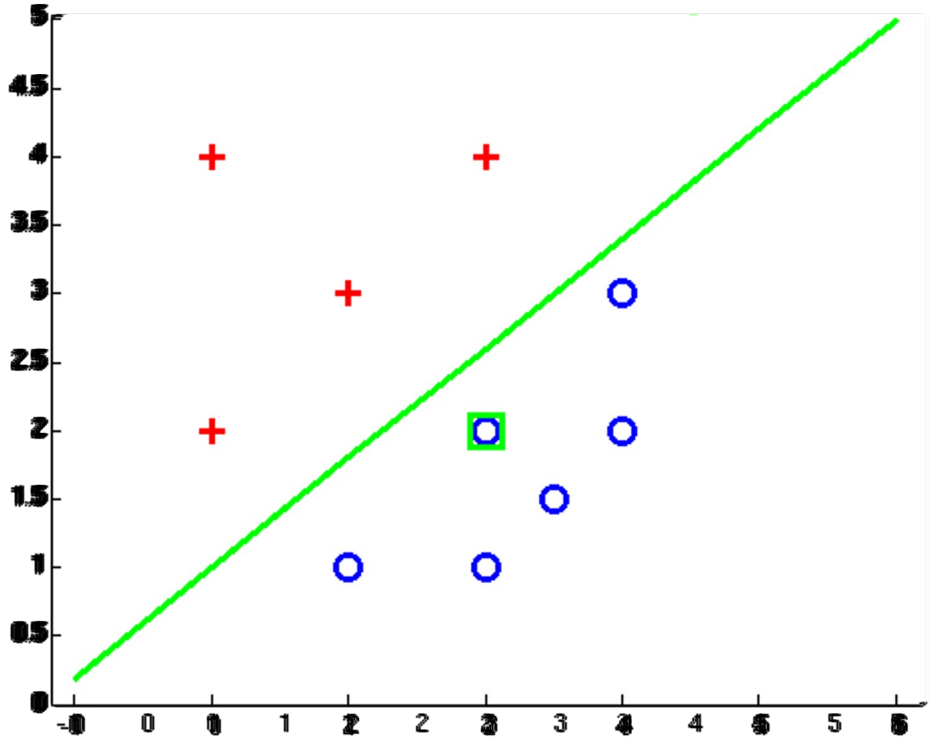
  - If correct (i.e., y=y*), no change!
  - If wrong: adjust the weight vector by adding or subtracting the feature vector. Subtract if y* is -1.

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



Examples: Perceptron

- Separable Case



Multiclass Decision Rule

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

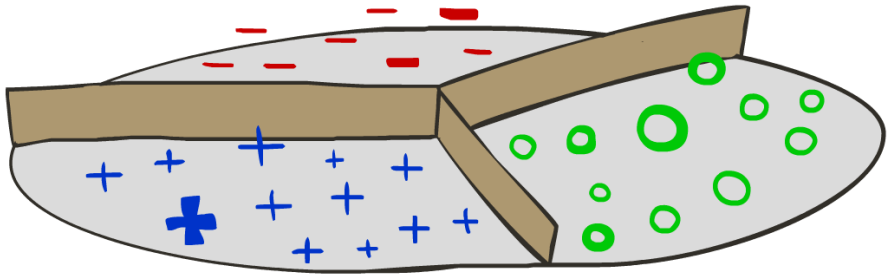
$$w_y$$

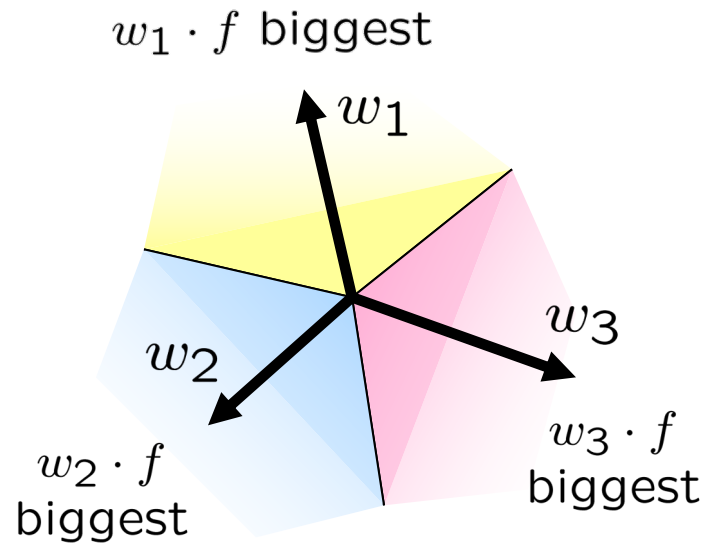
  - Score (activation) of a class y:

$$w_y \cdot f(x)$$

  - 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

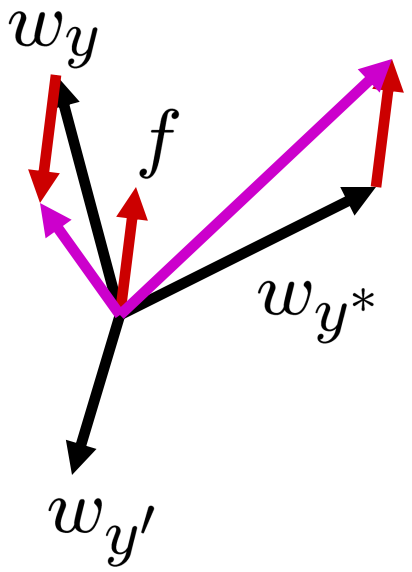
- Start with all weights = 0
- Pick up training examples one by one
- Predict with current weights

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

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

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

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



Example: Multiclass Perceptron

"win the vote"

"win the election"

"win the game"

w_{SPORTS}

```
BIAS  : 1
win   : 0
game  : 0
vote  : 0
the   : 0
...
```

$w_{POLITICS}$

```
BIAS  : 0
win   : 0
game  : 0
vote  : 0
the   : 0
...
```

w_{TECH}

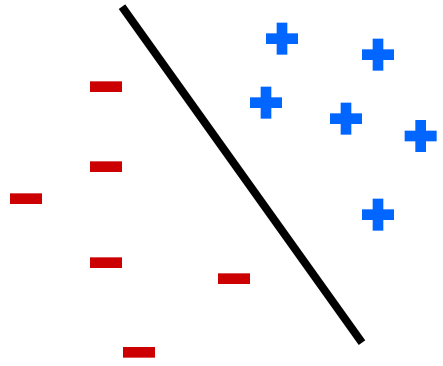
```
BIAS  : 0
win   : 0
game  : 0
vote  : 0
the   : 0
...
```

Properties of Perceptrons

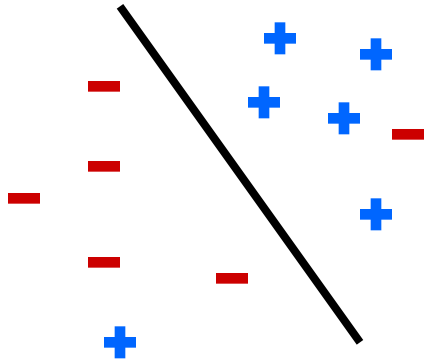
- Separability: true if some parameters get the training set perfectly correct
- Convergence: if the training is separable, perceptron will eventually converge (binary case)
- Mistake Bound: the maximum number of mistakes (binary case) related to the *margin* or degree of separability

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

Separable

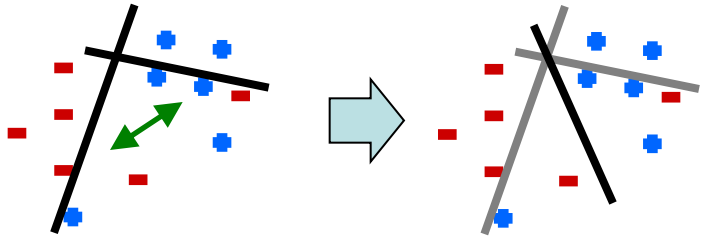


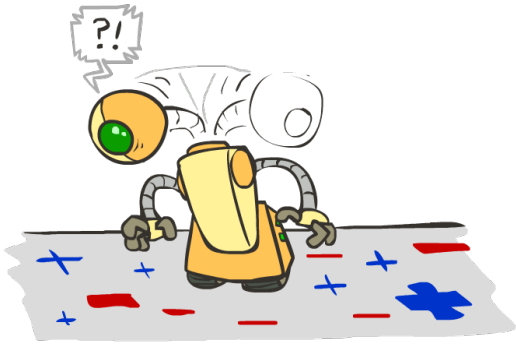
Non-Separable



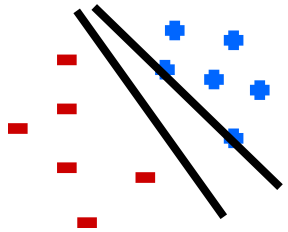
Problems with the Perceptron

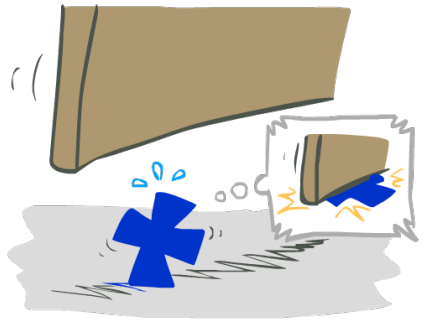
- Noise: if the data isn't separable, weights might thrash
  - Averaging weight vectors over time can help (averaged perceptron)



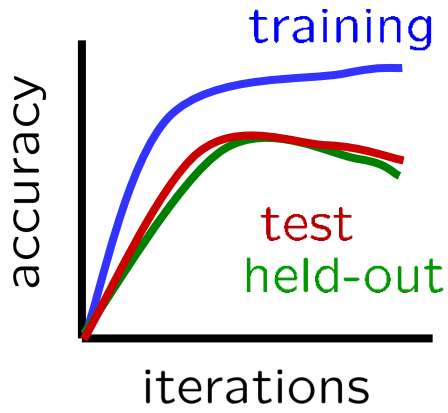


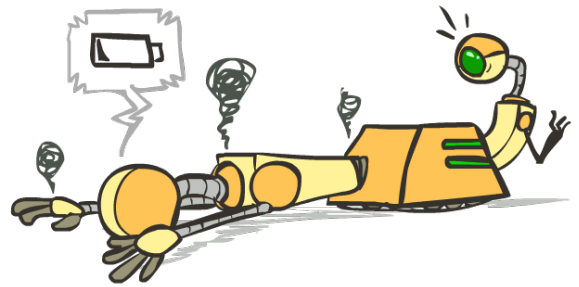
- Mediocre generalization: finds a "barely" separating solution



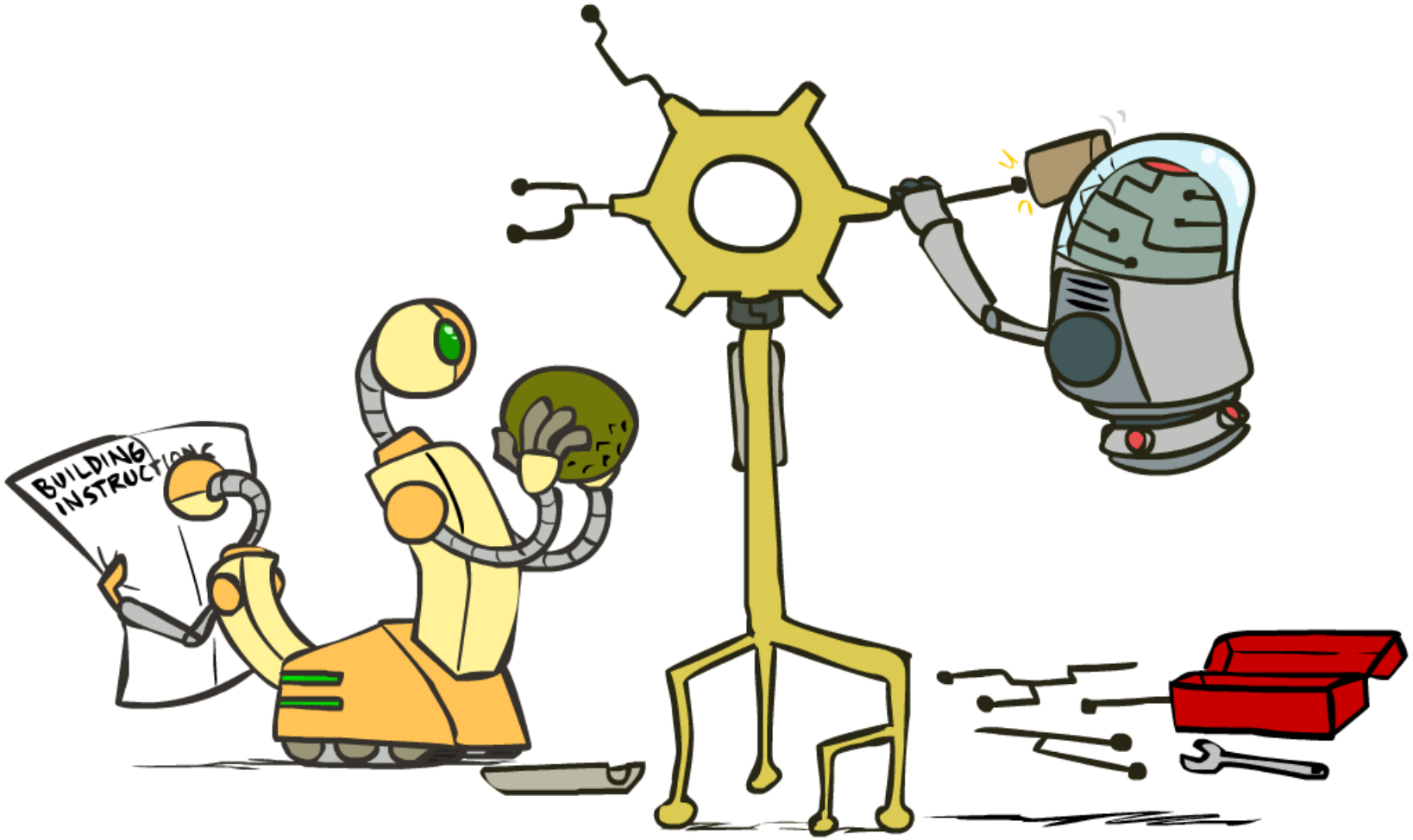


- Overtraining: test / held-out accuracy usually rises, then falls
  - Overtraining is a kind of overfitting



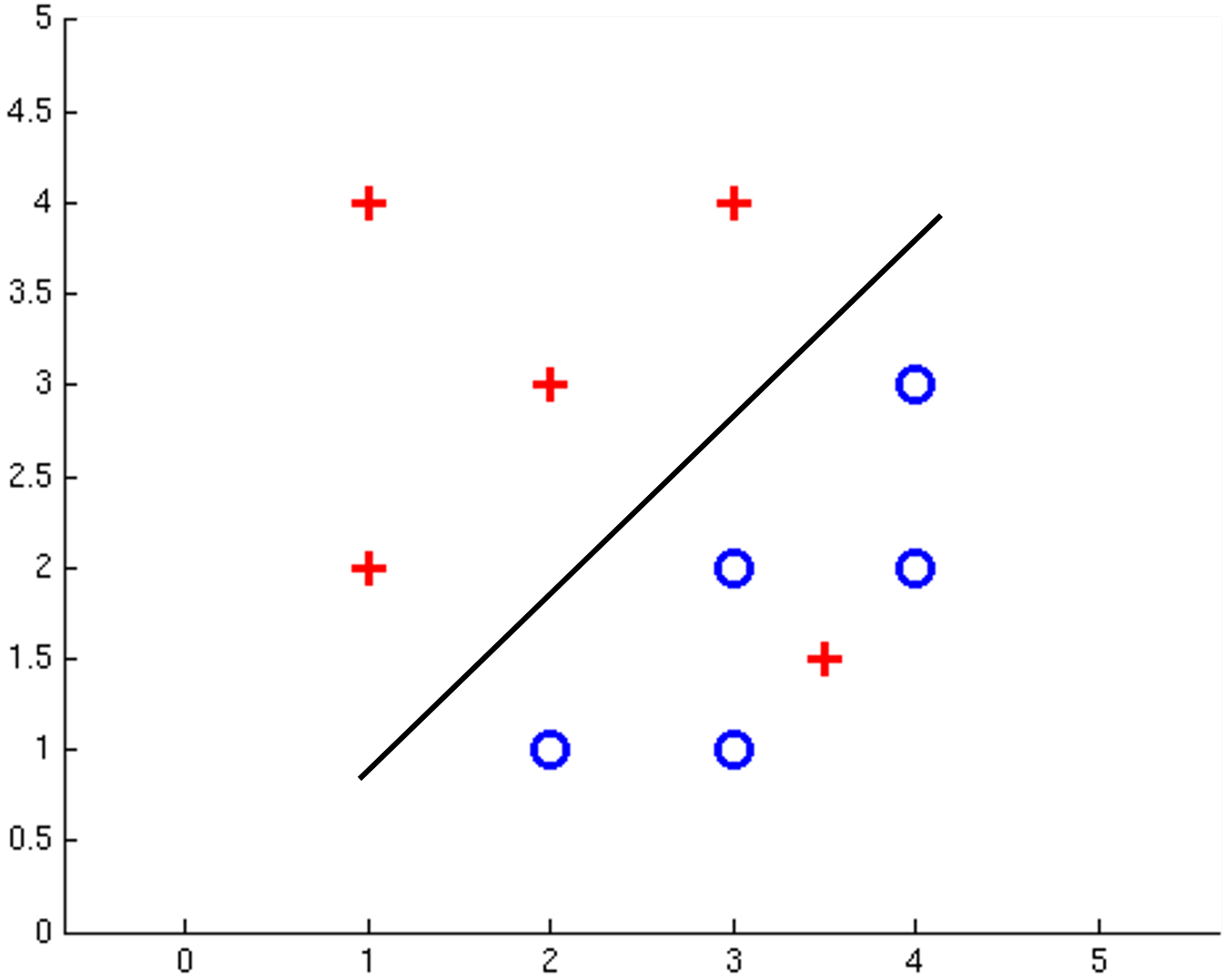


Improving the Perceptron

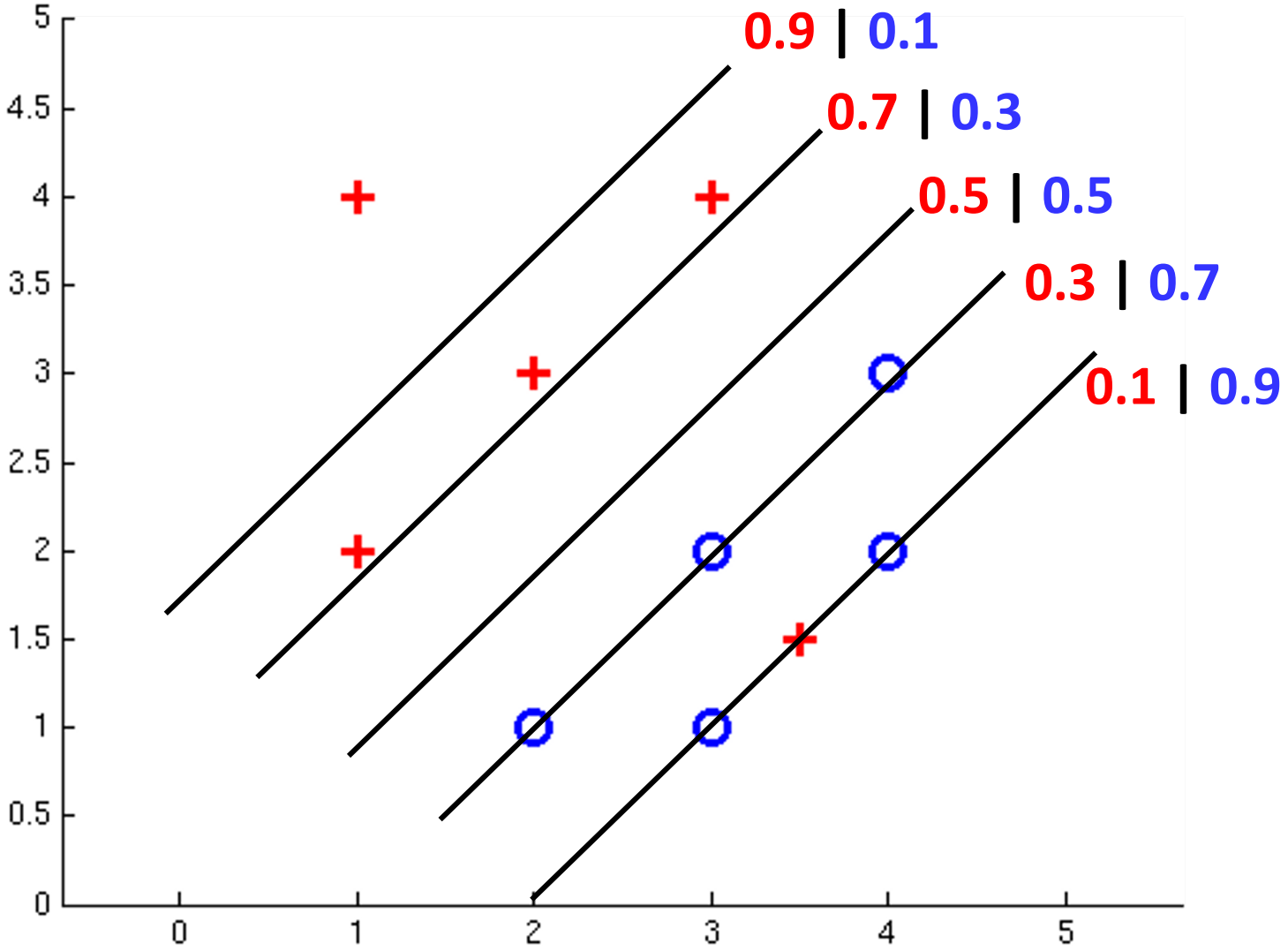


Non-Separable Case: Deterministic Decision

Even the best linear boundary makes at least one mistake



Non-Separable Case: Probabilistic Decision

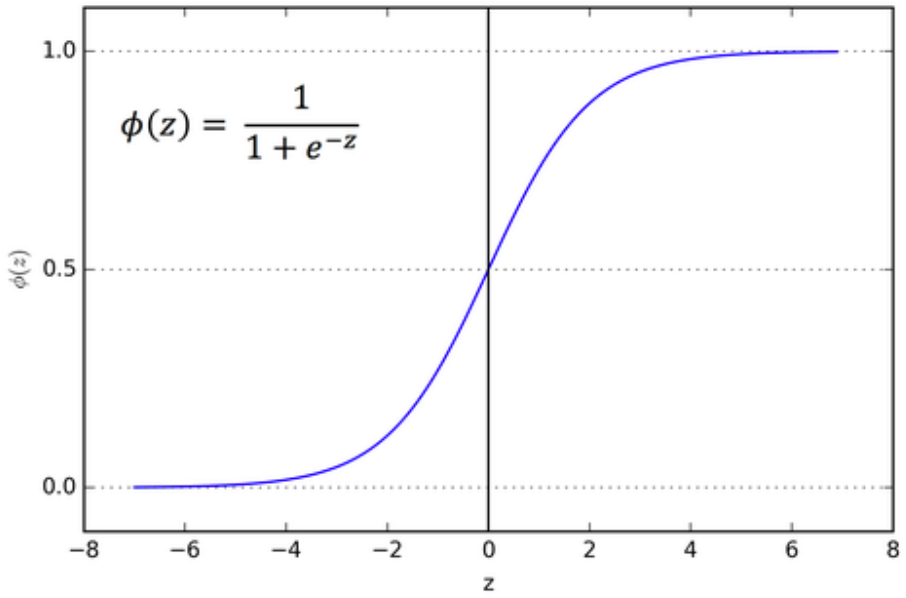


How to get probabilistic decisions?

- 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

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



Best w?

- Maximum likelihood estimation:

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

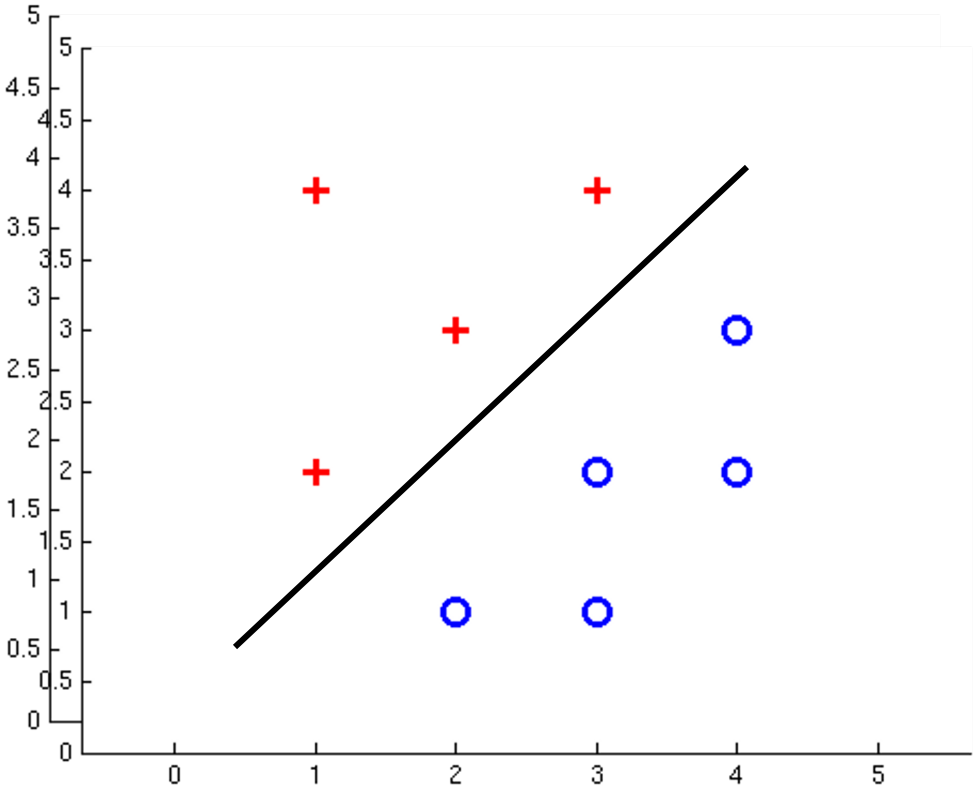
with:

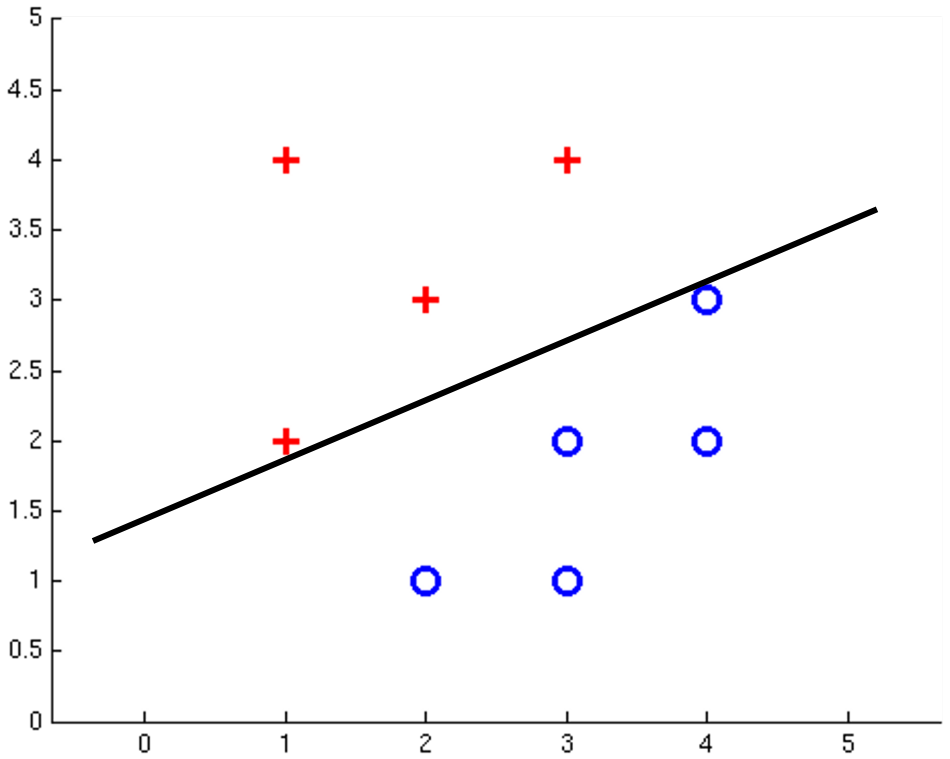
$$P(y^{(i)} = +1|x^{(i)};w) = \frac{1}{1+e^{-w\cdot f(x^{(i)})}}$$

$$P(y^{(i)} = -1|x^{(i)};w) = 1 - \frac{1}{1+e^{-w\cdot f(x^{(i)})}}$$

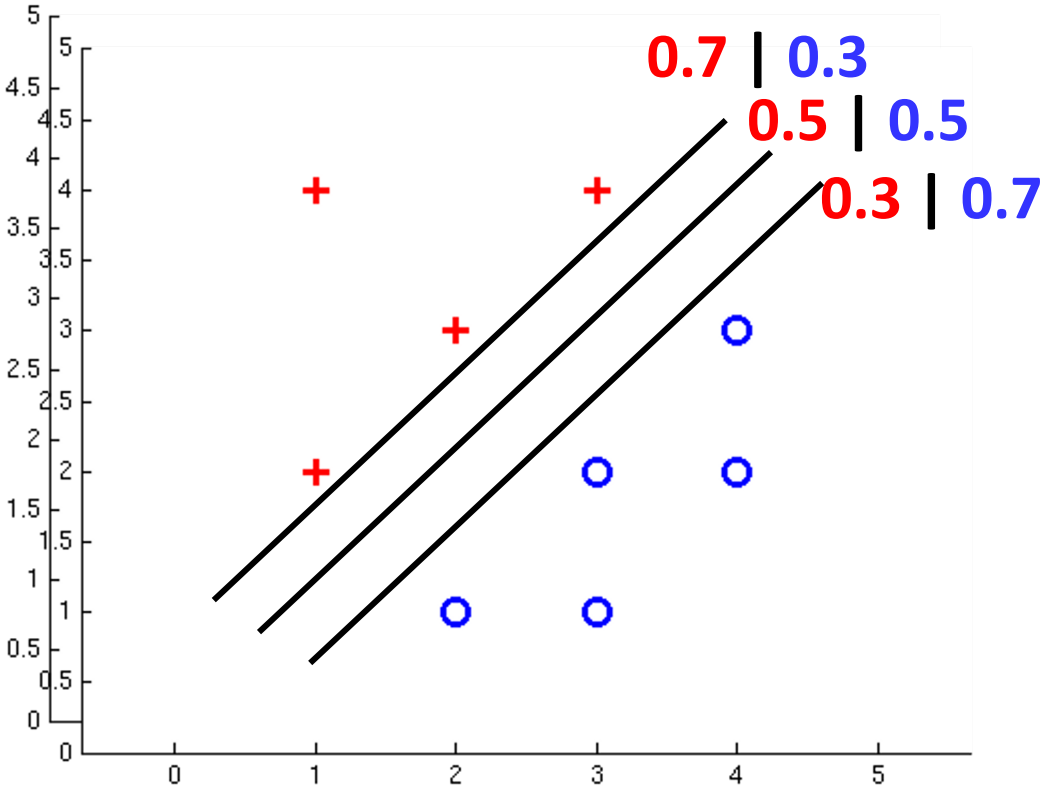
= Logistic Regression

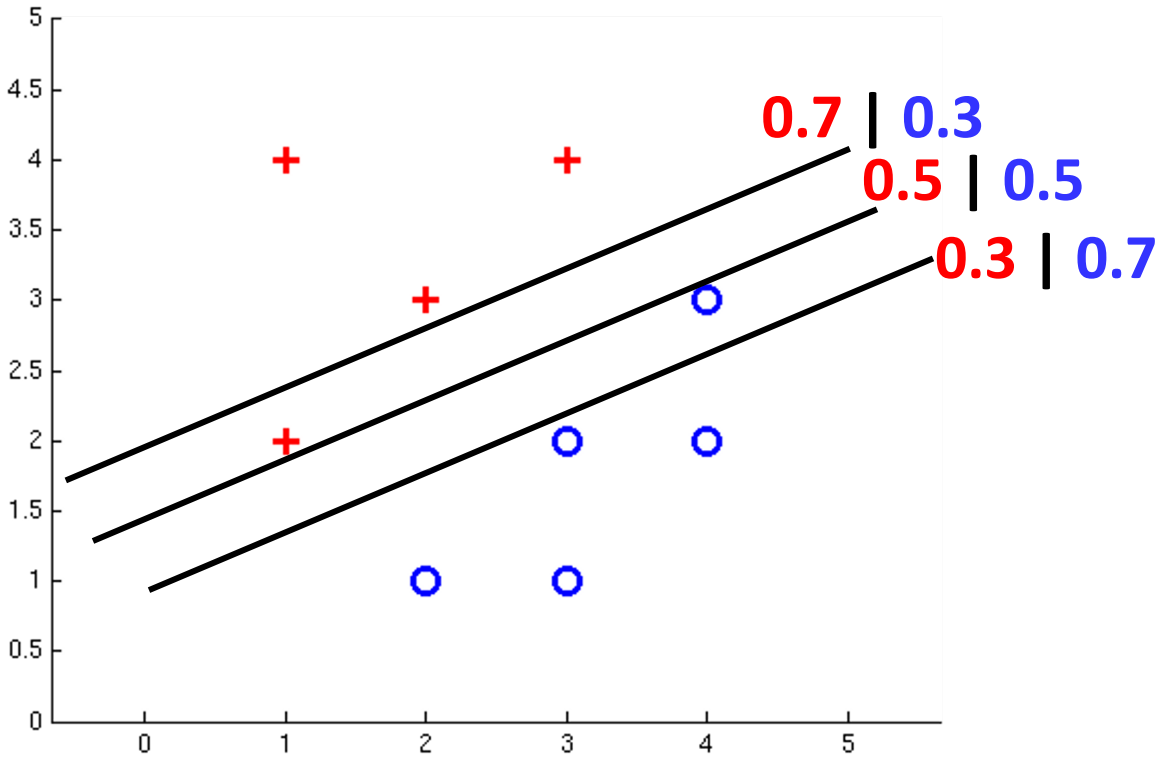
Separable Case: Deterministic Decision – Many Options





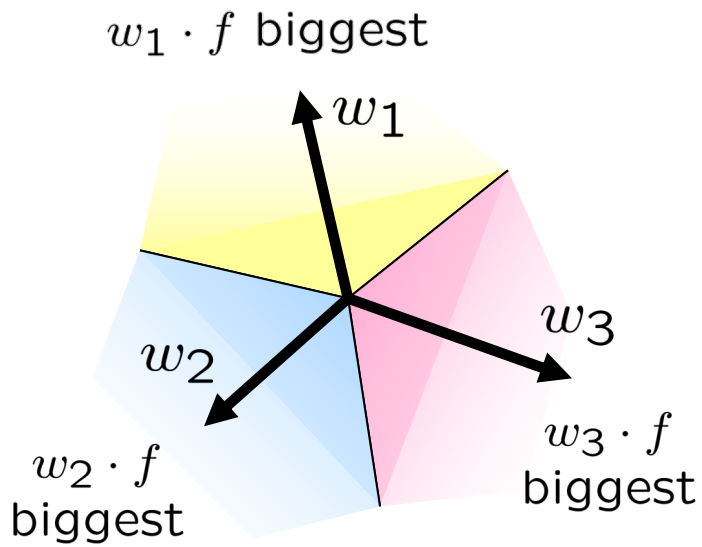
Separable Case: Probabilistic Decision – Clear Preference





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?

$$z_1, z_2, z_3 \rightarrow \frac{e^{z_1}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_2}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}}$$

original activations

softmax activations

Best w?

- Maximum likelihood estimation:

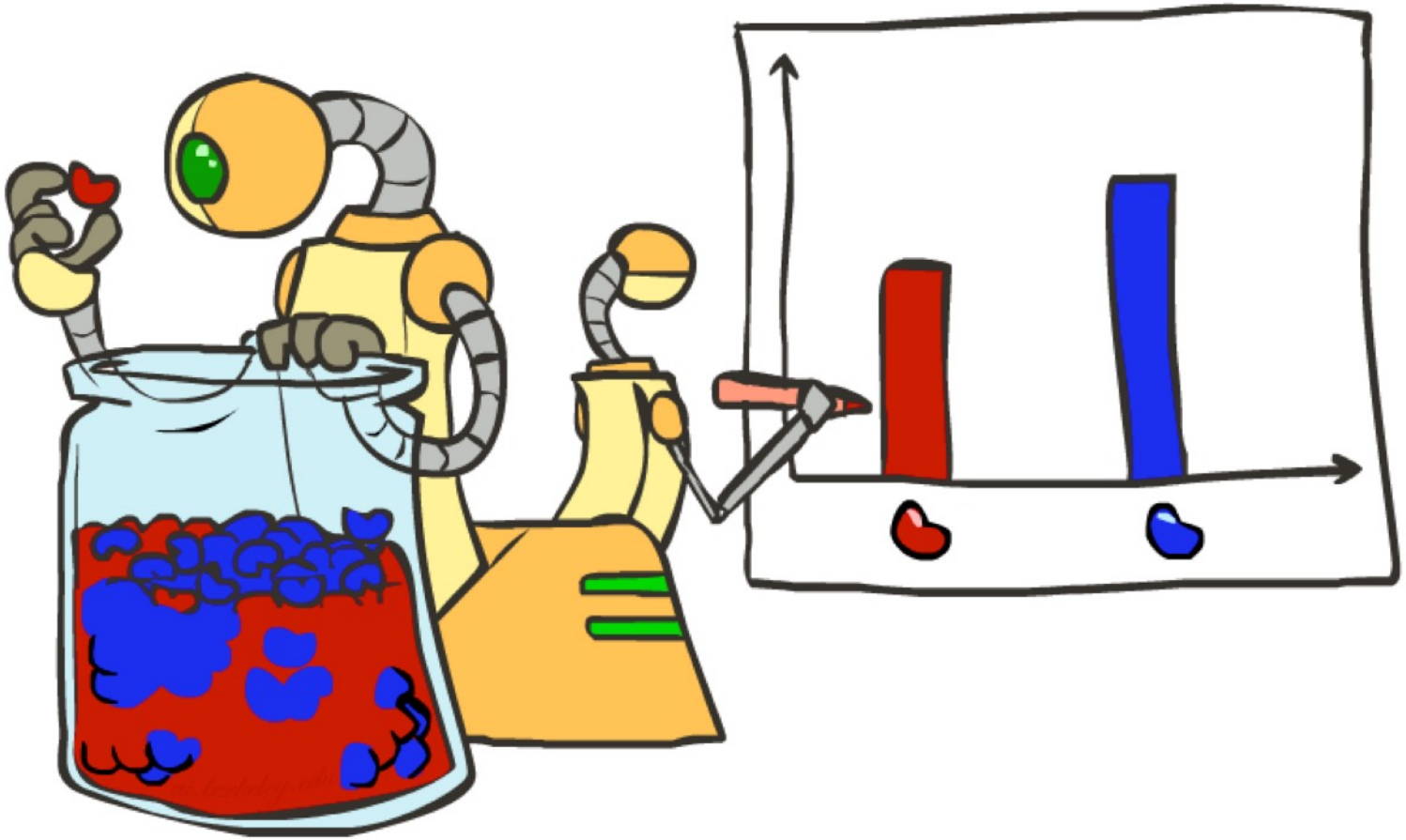
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

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

Maximum Likelihood Estimation



Parameter Estimation with Maximum Likelihood

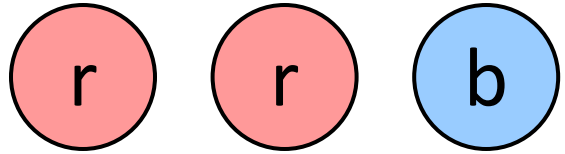
- Estimating the distribution of a random variable
- Use training data (learning!)
  - For each outcome x, look at the **empirical rate** of that value:

$$\mathrm{P}_{ML} = \frac{\mathrm{count}(x)}{\text{total samples}}$$

- Example: probability of x=red given the training data:

$$\mathrm{P}_{ML}(r) = \frac{2}{3}$$

x	red	blue
$P_\theta(x)$	θ	$1-\theta$



- This estimate maximizes the **likelihood of the data** for the parametric model:

$$L(\theta) = \mathrm{P}(\mathrm{r}, \mathrm{r}, \mathrm{b} \mid \theta) = \mathrm{P}_\theta(r) \cdot \mathrm{P}_\theta(r) \cdot \mathrm{P}_\theta(b)$$
$$= \theta^2 \cdot (1-\theta)$$

Parameter Estimation with Maximum Likelihood

- Likelihood function:

$$L(\theta) = \mathrm{P}(\,\mathrm{r}, \mathrm{r}, \mathrm{b} \mid \theta\,) = \mathrm{P}_\theta(r) \cdot \mathrm{P}_\theta(r) \cdot \mathrm{P}_\theta\,(b)$$
$$= \theta^2 \cdot (1-\theta)$$
$$= \theta^2 - \theta^3$$

- MLE: find the θ that maximizes data likelihood

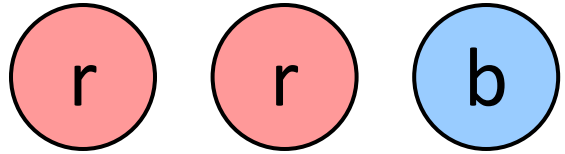
$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, L(\theta)$$

- Approach: take derivatives and set to 0

$$\frac{\partial L(\theta)}{\partial \theta} = 2\theta - 3\theta^2$$
$$= \theta(2 - 3\theta)$$

- Find the maximum at $\theta = \frac{2}{3}$

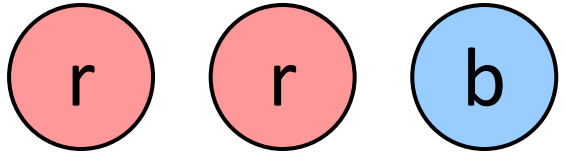
x	red	blue
$P_\theta(x)$	θ	$1-\theta$



Parameter Estimation (General Case)

- **Model**:

x	red	blue
$P_\theta(x)$	θ	$1-\theta$



- **Data**: draw N balls. N_r come up red, N_b come up blue
  - Dataset: $D = \{x_1, \ldots, x_n\}$
  - Ball draws are independent and identically distributed (i.i.d.):

$$P(D \mid \theta) = \prod_i P(x_i \mid \theta) = \prod_i P_\theta(x_i) = \theta^{N_r} \cdot (1-\theta)^{N_b}$$

- **Maximum likelihood estimation**: find θ that maximizes $P(D \mid \theta)$

$$\theta = \operatorname*{argmax}_\theta P(D \mid \theta) = \operatorname*{argmax}_\theta \log P(D \mid \theta)$$

  - Approach: take derivative and set to 0

Parameter Estimation (General Case)

- **Maximum likelihood estimation**: find θ that maximizes $P(\,D \mid \theta\,)$

$$\theta = \underset{\theta}{\operatorname{argmax}}\, P(\,D \mid \theta\,) = \underset{\theta}{\operatorname{argmax}} \log P(\,D \mid \theta\,)$$

$$\begin{aligned}\frac{\partial}{\partial\theta}\log P(\,D \mid \theta\,) &= \frac{\partial}{\partial\theta}\left[N_r \log(\theta) + N_b \log(1-\theta)\right] \\ &= N_r \frac{\partial}{\partial\theta}\log(\theta) + N_b \frac{\partial}{\partial\theta}\log(1-\theta) \\ &= N_r \frac{1}{\theta} - N_b \frac{1}{1-\theta} \\ &= 0\end{aligned}$$

Multiply by $\theta(1-\theta)$:

$$N_r(1-\theta) - N_b\theta = 0$$
$$N_r - \theta(N_r + N_b) = 0$$

$$\hat{\theta} = \frac{N_r}{N_r + N_b}$$

Example from Discussion 6B

1 Maximum Likelihood Estimation

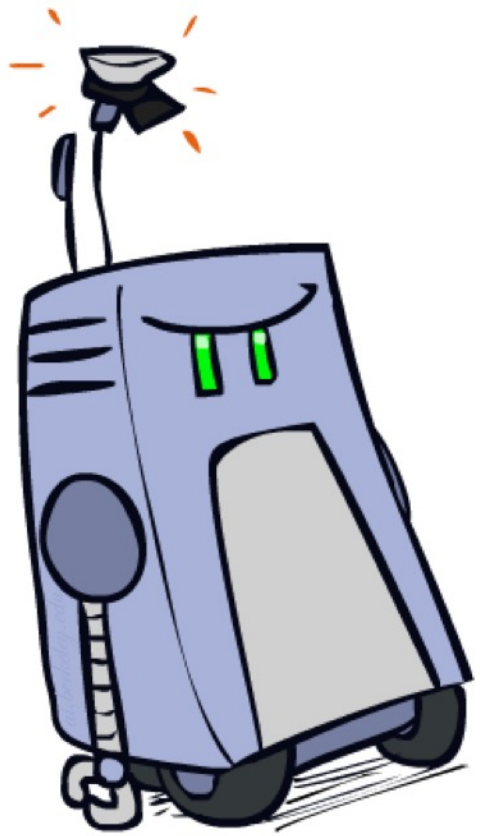
Recall that a Geometric distribution is a defined as the number of Bernoulli trials needed to get one success. $P(X = k) = p(1-p)^{k-1}$.
We observe the following samples from a Geometric distribution:
$x_1 = 5$, $x_2 = 8$, $x_3 = 3$, $x_4 = 5$, $x_5 = 7$
What is the maximum likelihood estimate for p?

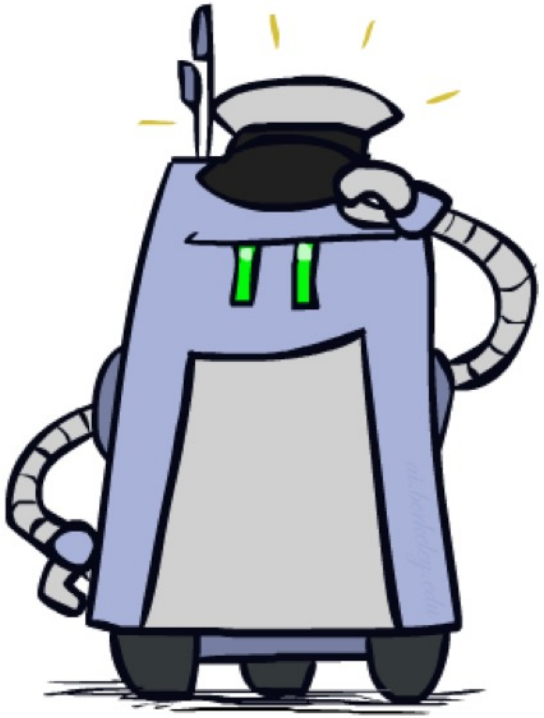
$$L(p) = P(X = x_1)P(X = x_2)P(X = x_3)P(X = x_4)P(X = x_5) \quad (1)$$
$$= P(X = 5)P(X = 8)P(X = 3)P(X = 5)P(X = 7) \quad (2)$$
$$= p^5(1-p)^{23} \quad (3)$$
$$\log(L(p)) = 5\log(p) + 23\log(1-p) \quad (4)$$
$$(5)$$

We must maximize the log-likelihood of p, so we will take the derivative, and set it to 0.

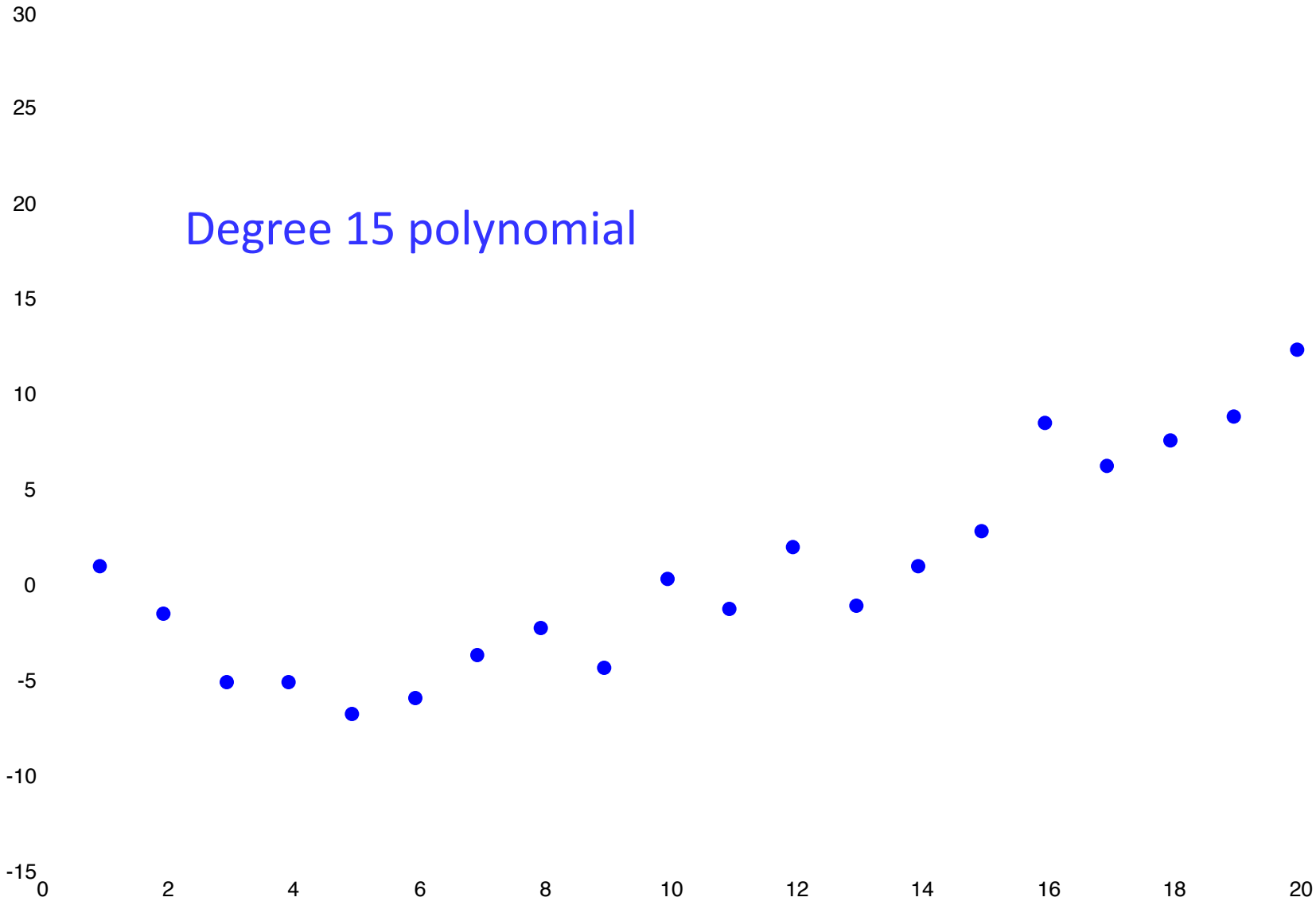
$$0 = \frac{5}{p} - \frac{23}{1-p} \quad (6)$$
$$p = 5/28 \quad (7)$$

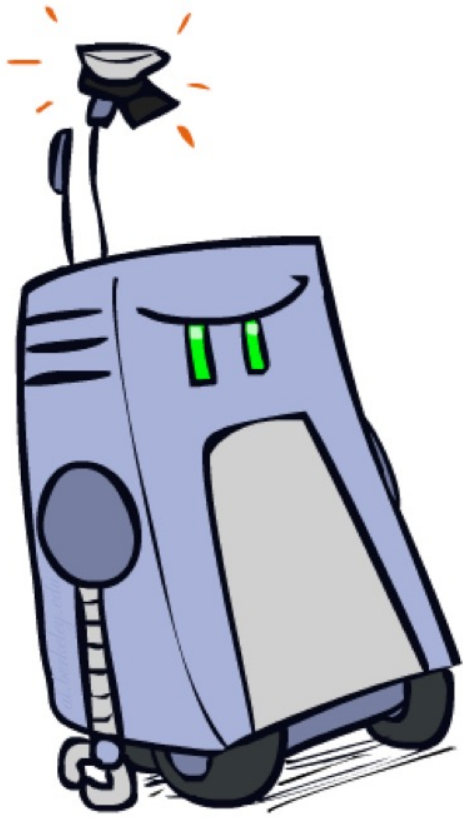
Regularization





Recall: Overfitting





Example: Overfitting

$P(\text{features}, C = 2)$

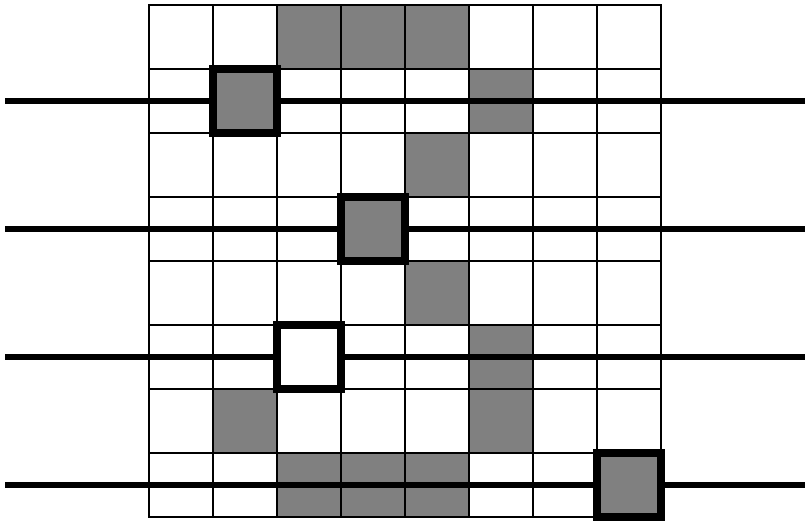
$P(C = 2) = 0.1$

$P(\text{on}|C = 2) = 0.8$

$P(\text{on}|C = 2) = 0.1$

$P(\text{off}|C = 2) = 0.1$

$P(\text{on}|C = 2) = 0.01$



$P(\text{features}, C = 3)$

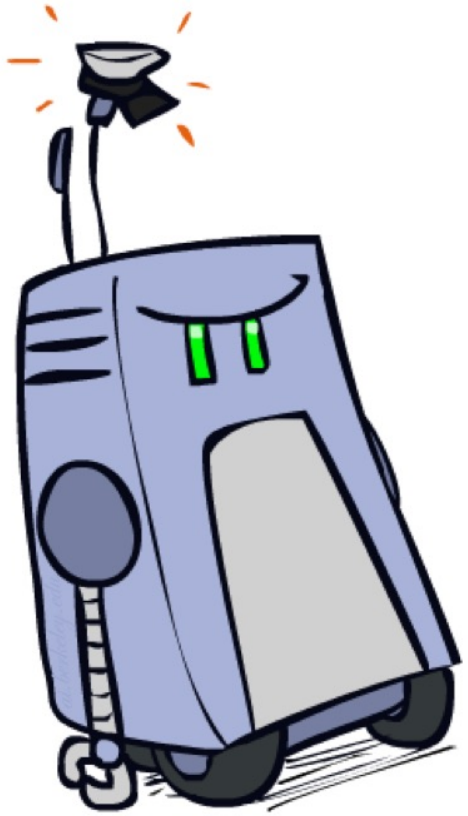
$P(C = 3) = 0.1$

$P(\text{on}|C = 3) = 0.8$

$P(\text{on}|C = 3) = 0.9$

$P(\text{off}|C = 3) = 0.7$

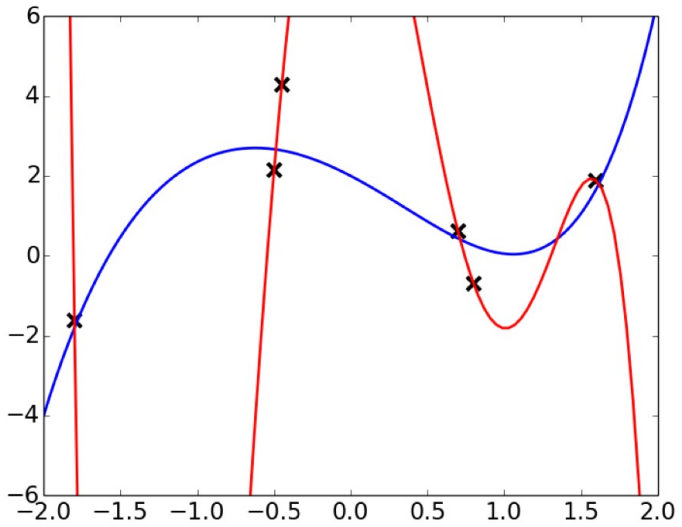
$P(\text{on}|C = 3) = 0.0$



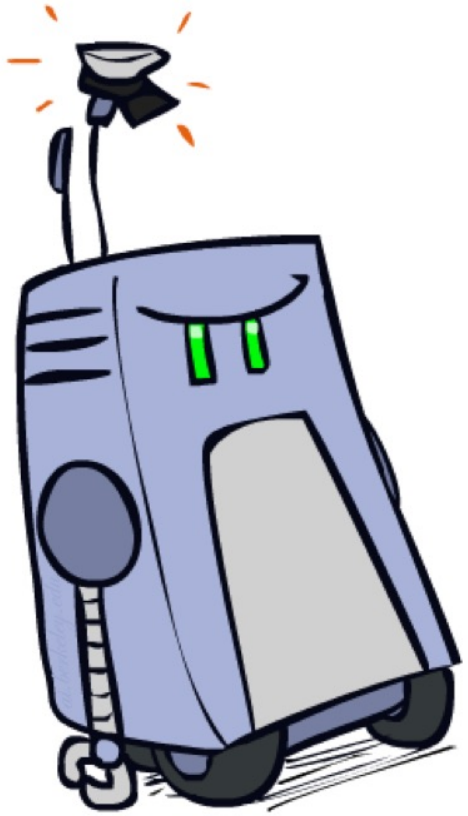
2 wins!!

Recall: Overfitting

- Observation: polynomials that overfit tend to have large coefficients



$$y = 0.1x^5 + 0.2x^4 + 0.75x^3 - x^2 - 2x + 2$$
$$y = -7.2x^5 + 10.4x^4 + 24.5x^3 - 37.9x^2 - 3.6x + 12$$



- Let's try to keep coefficients small!

Slide courtesy of Roger Grosse, Amir-massoud Farahmand, and Juan Carrasquilla (U Toronto)

L1 and L2 Regularization

- Previously:

$$\hat{w} = \arg\max_{w} \sum_{i=1}^{n} \log P\left(y^{(i)} \mid x^{(i)}; w\right)$$

- Now: add a penalty term to keep the weight vector small

L1
(aka lasso regression)

$$\hat{w} = \arg\max_{w} \sum_{i=1}^{n} \log P\left(y^{(i)} \mid x^{(i)}; w\right) - \alpha \sum_{i=1}^{n} |w_i|$$

L2
(aka ridge regression)

$$\hat{w} = \arg\max_{w} \sum_{i=1}^{n} \log P\left(y^{(i)} \mid x^{(i)}; w\right) - \alpha \sum_{i=1}^{n} w_i^2$$