CSEP 573: Artificial Intelligence

Machine Learning

slides adapted from
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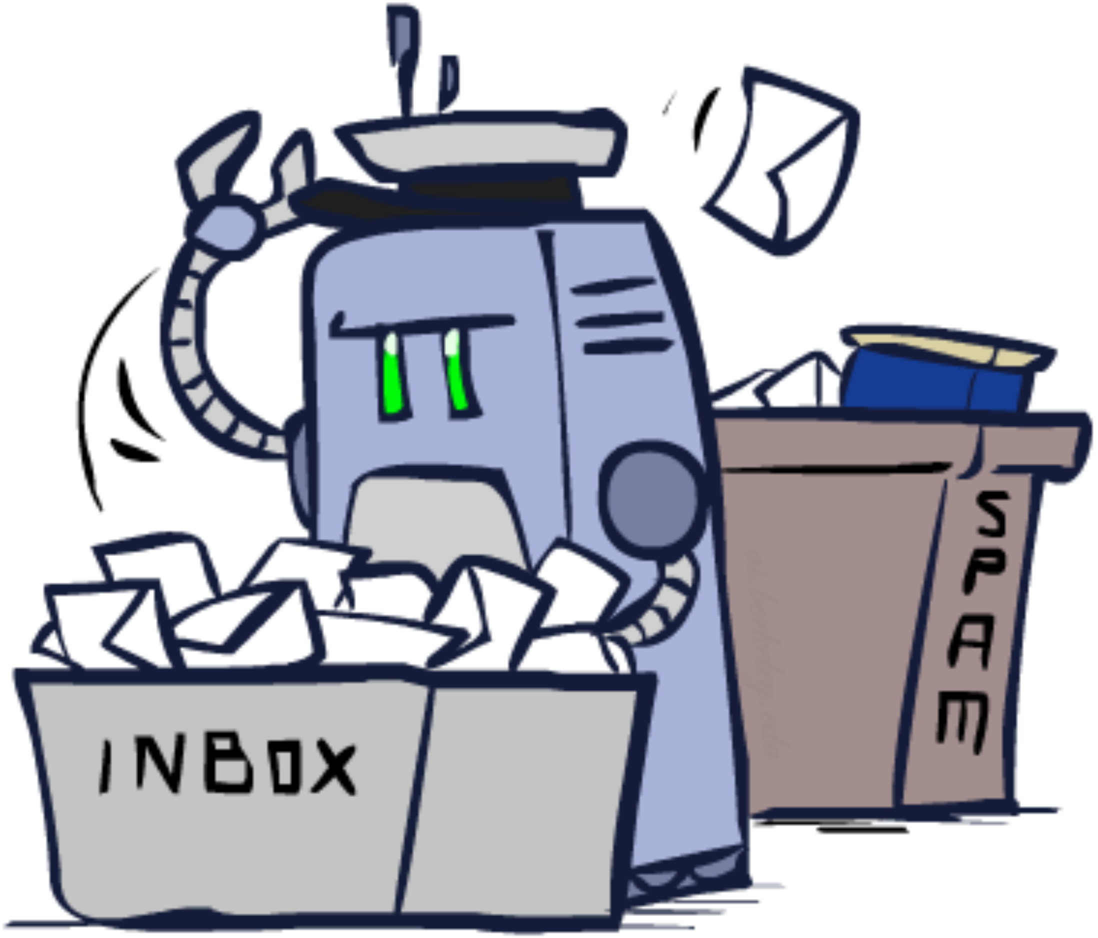
Machine Learning

- 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)

- 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
  - …

> 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

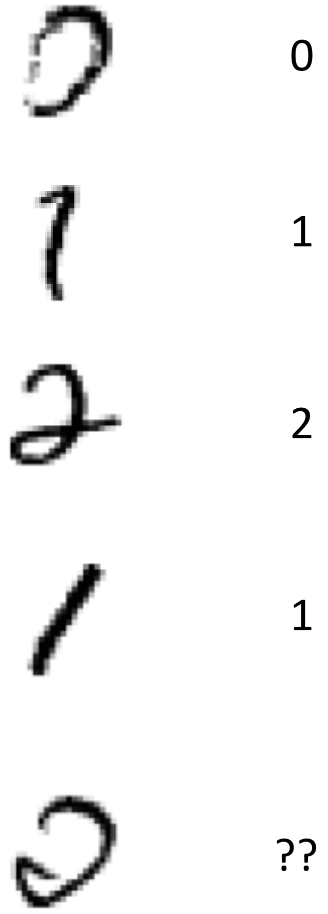
> Ok, Iknow this is blatantly OT but I'm beginning to go insane. Had an old Dell Dimension XPS sitting in the corner and decided to put it to use, I know it was working pre being stuck in the corner, but when I plugged it in, hit the power nothing happened.

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

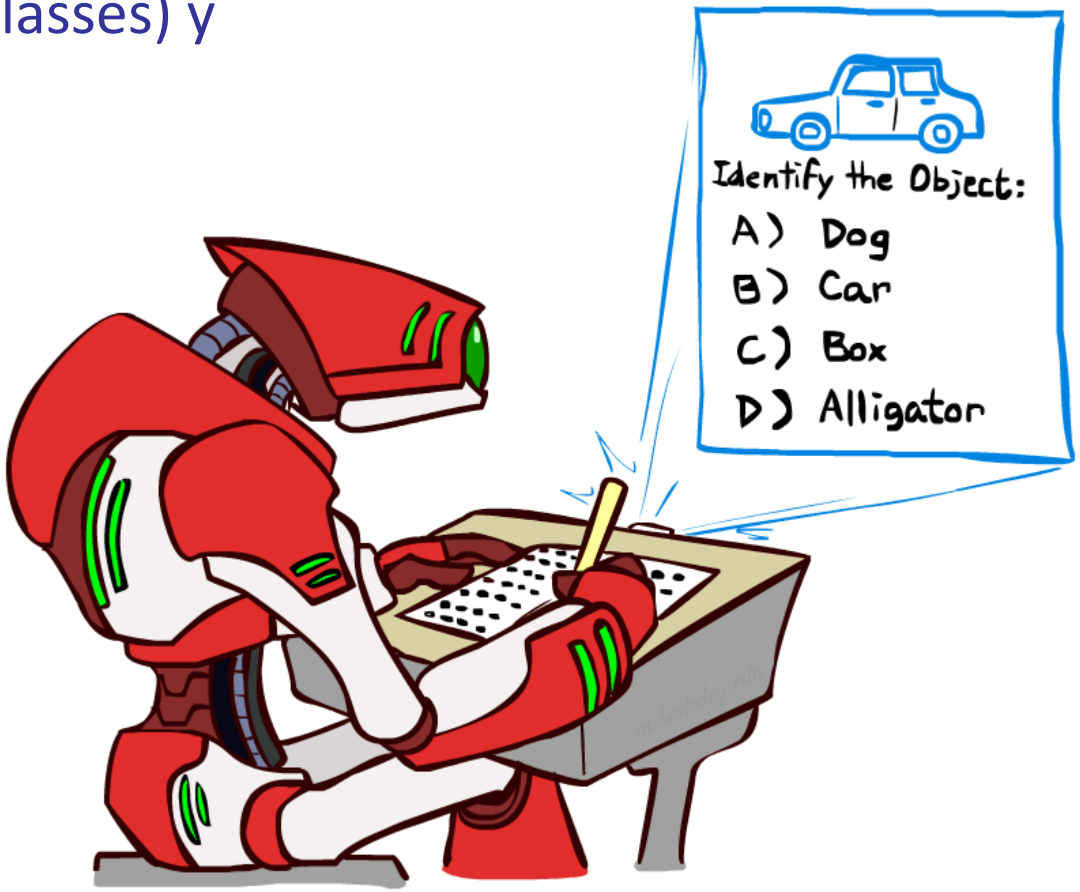
- Features: The attributes used to make the digit decision
  - Pixels: (6,8)=ON
  - Shape Patterns: NumComponents, AspectRatio, NumLoops
  - …



Other Classification Tasks

- Classification: given inputs x, predict labels (classes) y

- Examples:
  - Spam detection (input: document, classes: spam / ham)
  - OCR (input: images, classes: characters)
  - Medical diagnosis (input: symptoms, classes: diseases)
  - Automatic essay grading (input: document, classes: grades)
  - Fraud detection (input: account activity, classes: fraud / no fraud)
  - Customer service email routing
  - … many more



- Classification is an important commercial technology!

Model-Based Classification

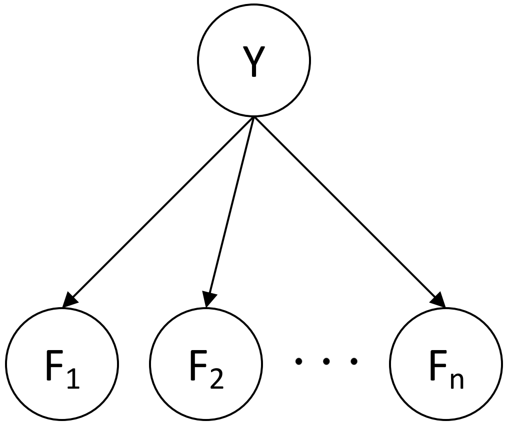
Model-Based Classification

- Model-based approach
  - Build a model (e.g. Bayes' net) where both the label and 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

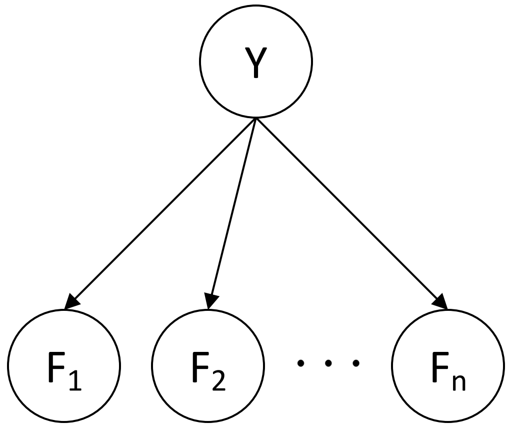
- A general Naive Bayes model:

|Y| parameters

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

|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

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

$$\xrightarrow{+} \; P(f_1 \dots f_n)$$

  - Step 2: sum to get probability of evidence

$$\Downarrow$$

  - Step 3: normalize by dividing Step 1 by Step 2

$$P(Y|f_1 \dots f_n)$$

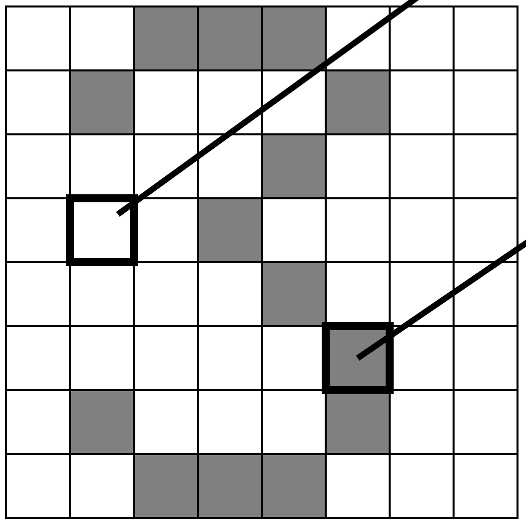
General Naïve Bayes

- 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

A Spam Filter

- Naïve Bayes spam filter
- Data:
  - Collection of emails, labeled spam or ham
  - Note: someone has to hand label all this data!
  - Split into training, held-out, test sets
- Classifiers
  - Learn on the training set
  - (Tune it on a held-out set)
  - Test it on new emails

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Naïve Bayes for Text

- Bag-of-words Naïve Bayes:
  - Features: W_i is the word at positon 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: $P(Y, W_1 \ldots W_n) = P(Y) \prod_i P(W_i|Y)$

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: $P(Y, W_1 \ldots W_n) = P(Y) \prod_i P(W_i|Y)$
- 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
...	

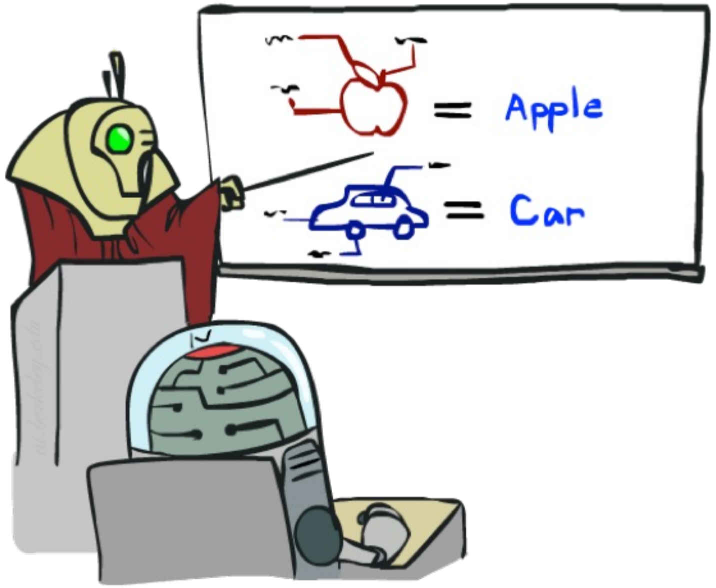
- Where do these tables come from?

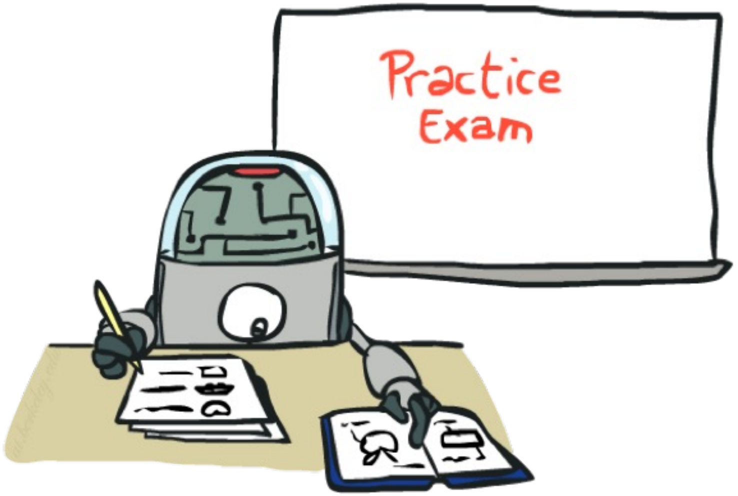
Spam Example

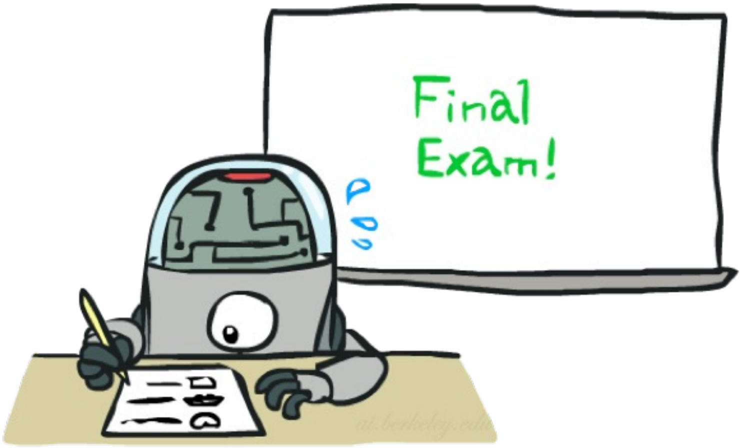
Word	P(w|spam)	P(w|ham)	Tot Spam	Tot Ham
(prior)	0.33333	0.66666	-1.1	-0.4

P(spam | w) = 98.9

Training and Testing







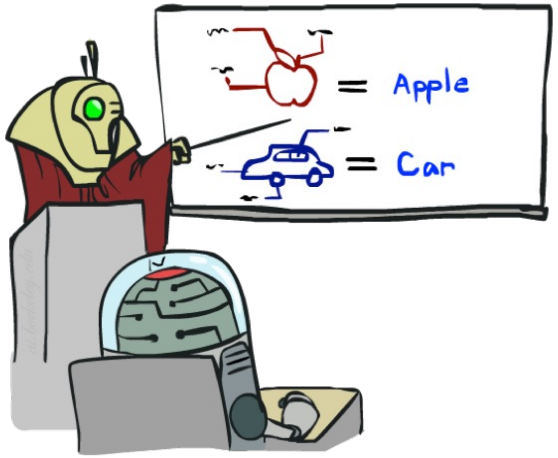
Important Concepts

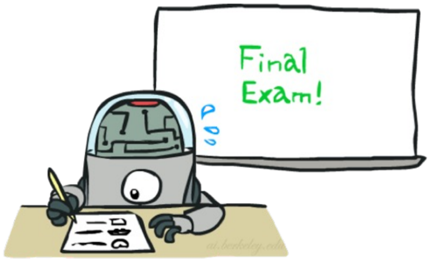
- Data: labeled instances, e.g. emails marked spam/ham
  - Training set
  - Held out set
  - Test set
- Features: attribute-value pairs which characterize each x
- Experimentation cycle
  - Learn parameters (e.g. model probabilities) on training set
  - (Tune hyperparameters on held-out set)
  - Compute accuracy of test set
  - Very important: never "peek" at the test set!
- Evaluation
  - 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

Training Data

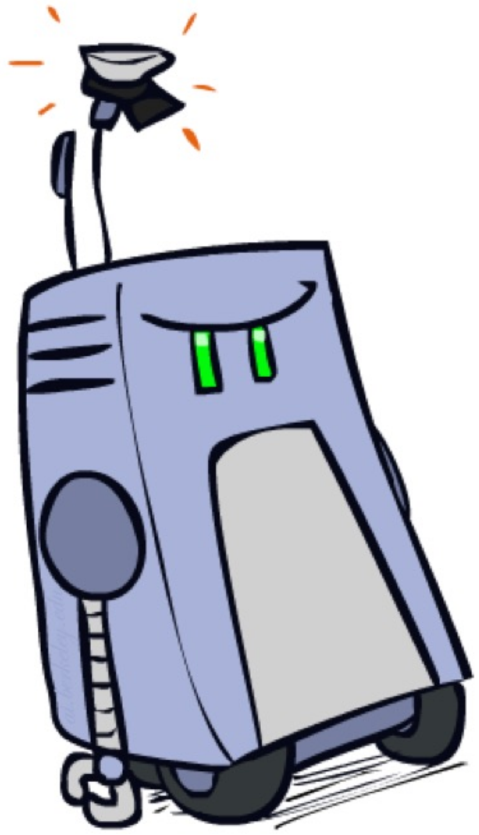
Held-Out Data

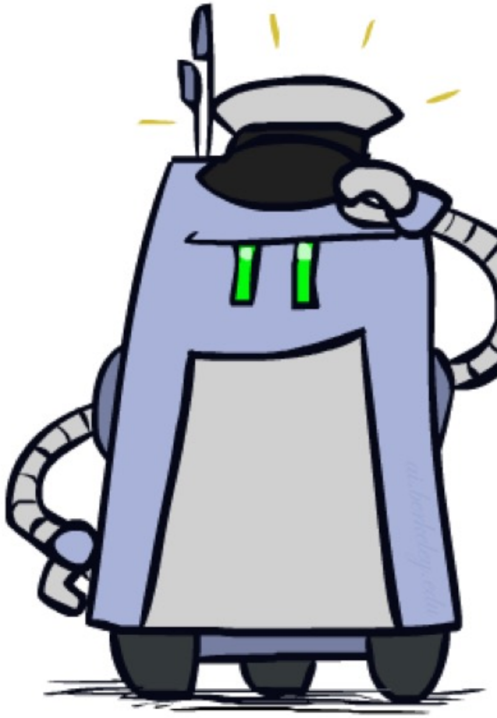
Test Data



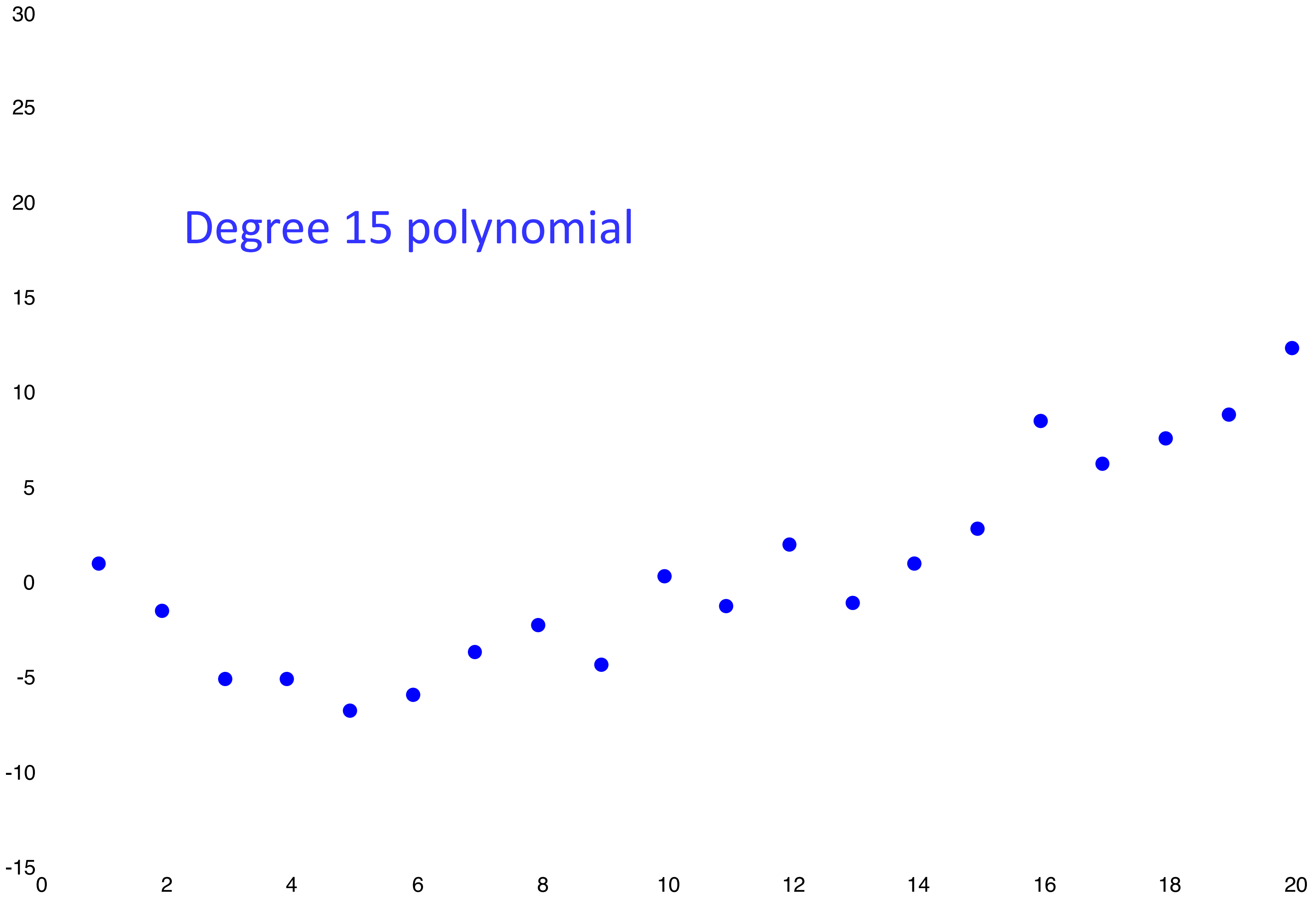


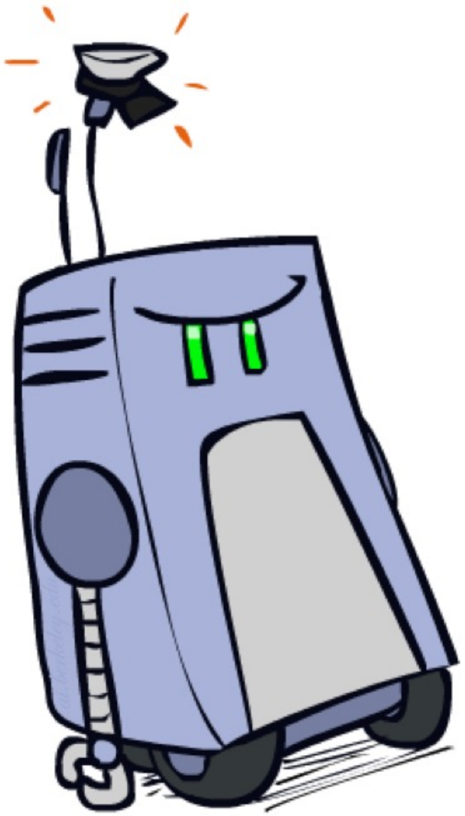
Generalization and Overfitting





Overfitting





Example: Overfitting

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

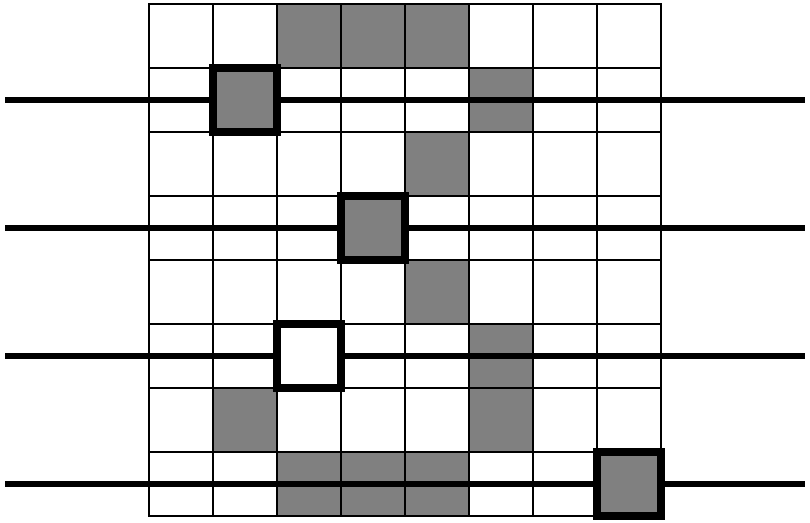
$P(C = 2) = 0.1$

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

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

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

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



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

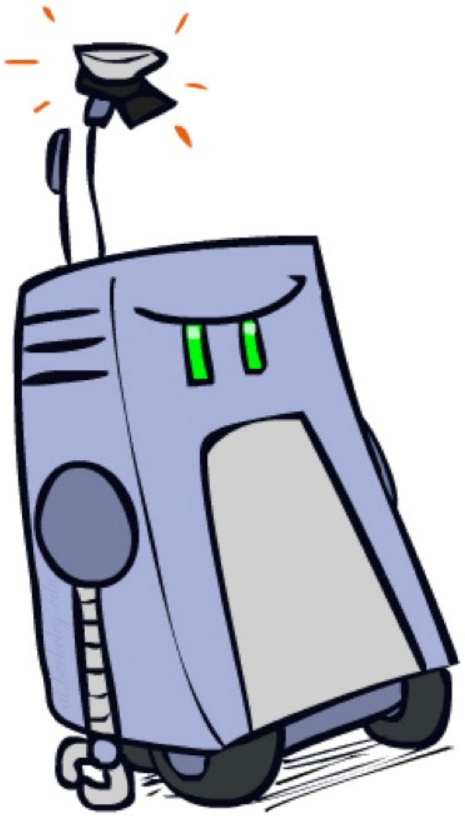
$P(C = 3) = 0.1$

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

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

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

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



2 wins!!

Example: Overfitting

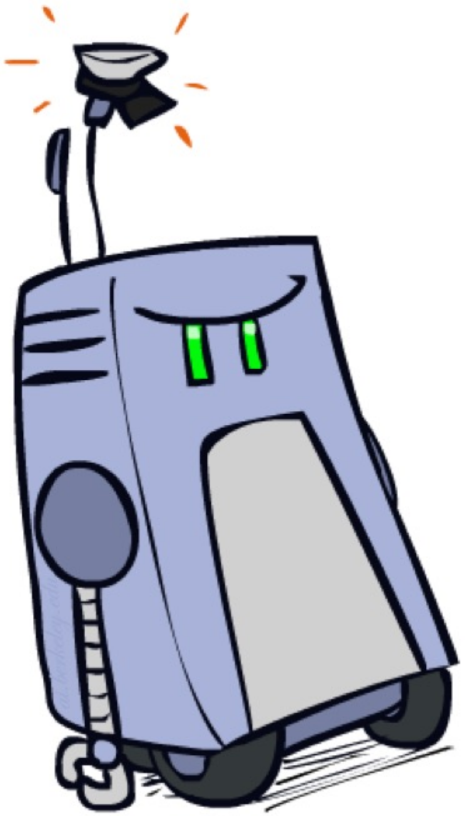
- Posteriors determined by *relative* probabilities (odds ratios):

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

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?

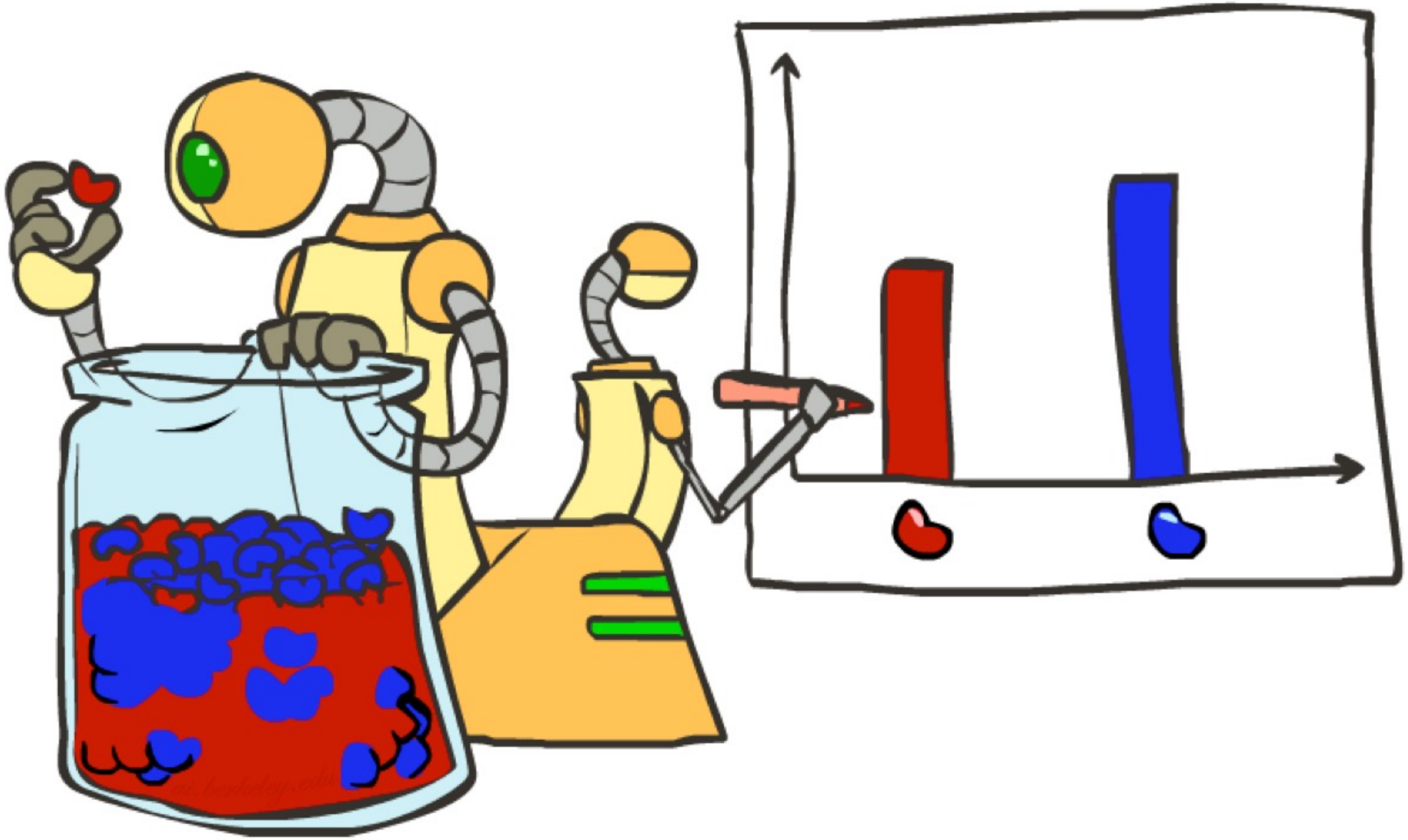
Generalization and Overfitting

- 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

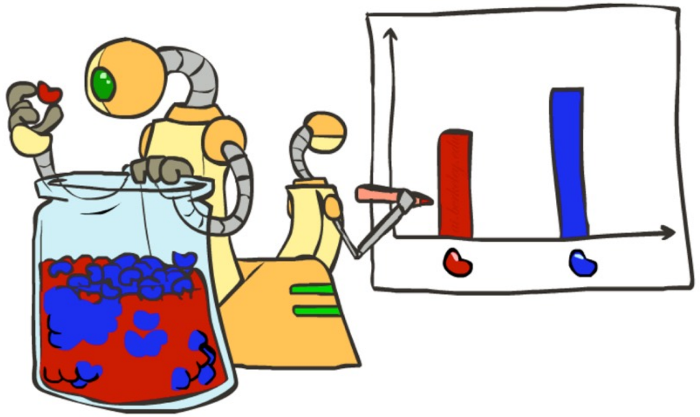
- As an extreme case, imagine using the entire email as the only feature
  - Would get the training data perfect (if deterministic labeling)
  - Wouldn't *generalize* at all
  - Just making the bag-of-words assumption gives us some generalization, but isn't enough

- 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:

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

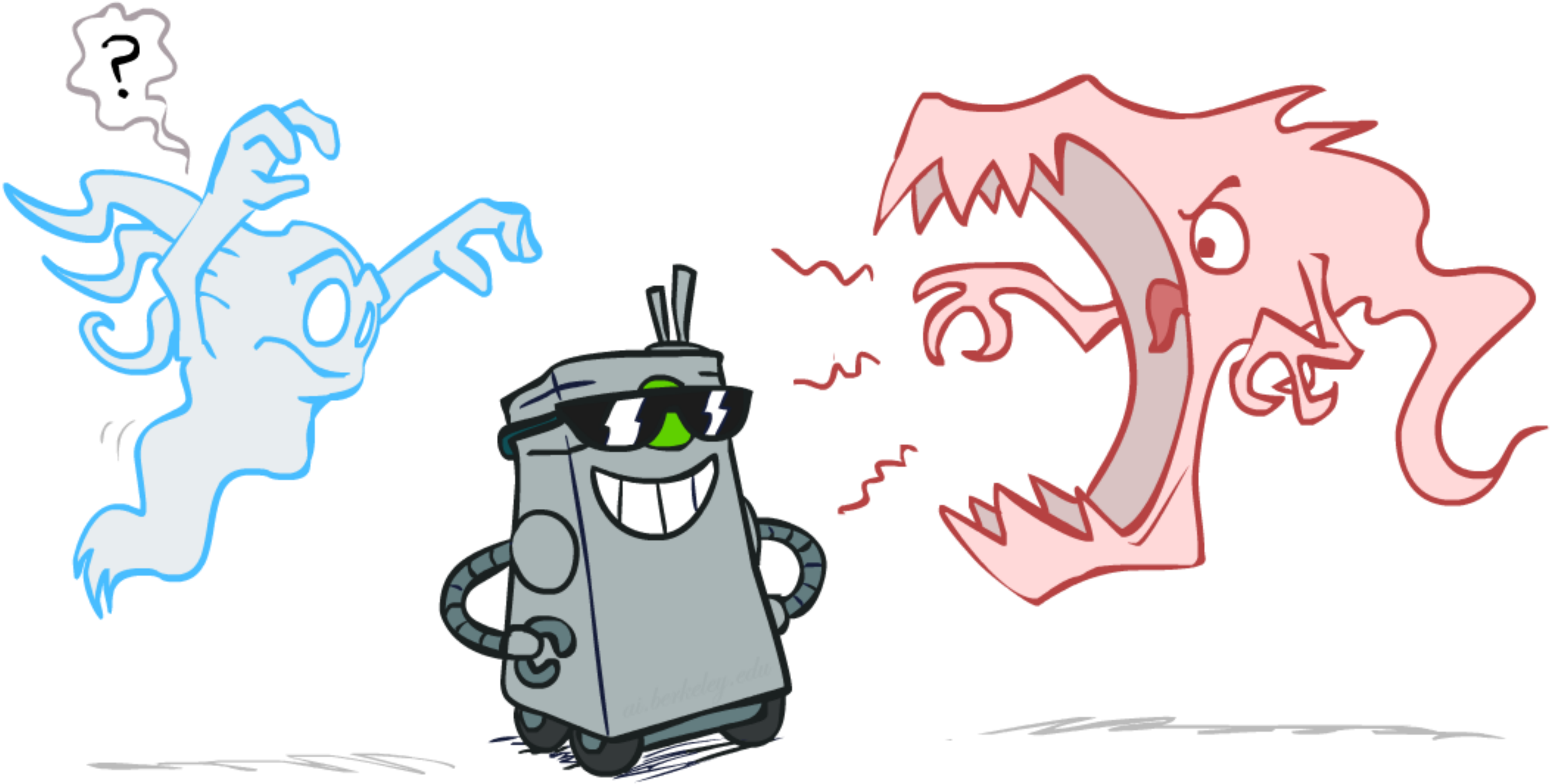
r r b

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

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

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

Smoothing



Maximum Likelihood?

- Relative frequencies are the maximum likelihood estimates

$$\theta_{ML} = \arg\max_{\theta} P(\mathbf{X}|\theta) = \arg\max_{\theta} \prod_i P_{\theta}(X_i)$$

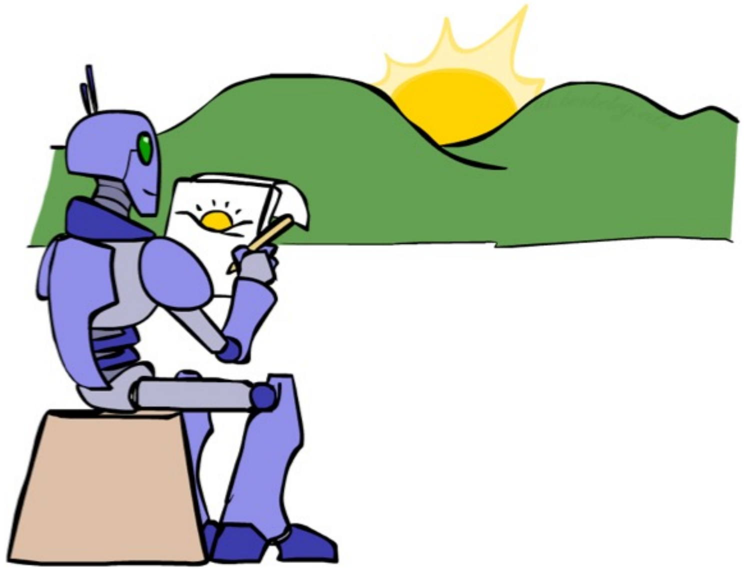
$$\Rightarrow \quad P_{\mathsf{ML}}(x) = \frac{\mathsf{count}(x)}{\mathsf{total\ samples}}$$

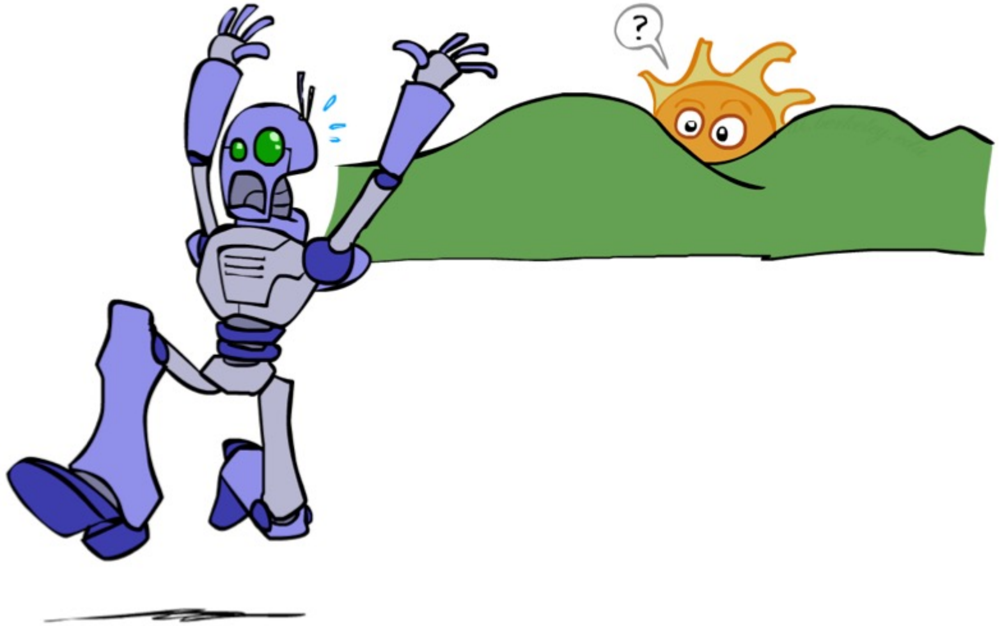
- Another option is to consider the most likely parameter value given the data

$$\begin{aligned}\theta_{MAP} &= \arg\max_{\theta} P(\theta|\mathbf{X}) \\ &= \arg\max_{\theta} P(\mathbf{X}|\theta)P(\theta)/P(\mathbf{X}) \\ &= \arg\max_{\theta} P(\mathbf{X}|\theta)P(\theta)\end{aligned}$$

$\Rightarrow$????

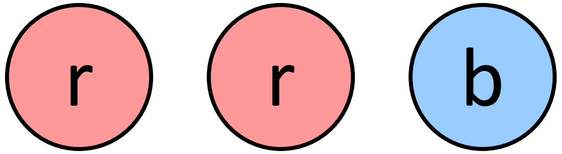
Unseen Events





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 ML class)

Laplace Smoothing

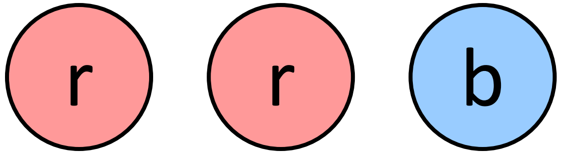
- Laplace's estimate (extended):
  - Pretend you saw every outcome k extra times

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

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

- Laplace for conditionals:
  - Smooth each condition independently:

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



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

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

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

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 advances ML/NLP classes

Real NB: Smoothing

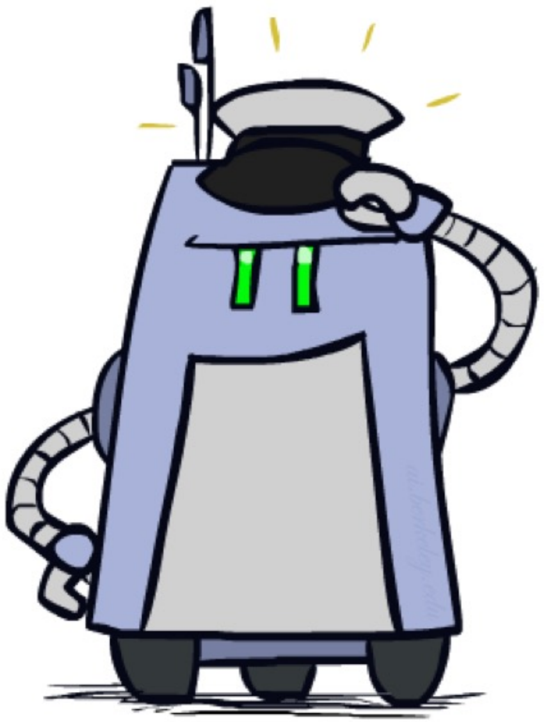
- For real classification problems, smoothing is critical
- New odds ratios:

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

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

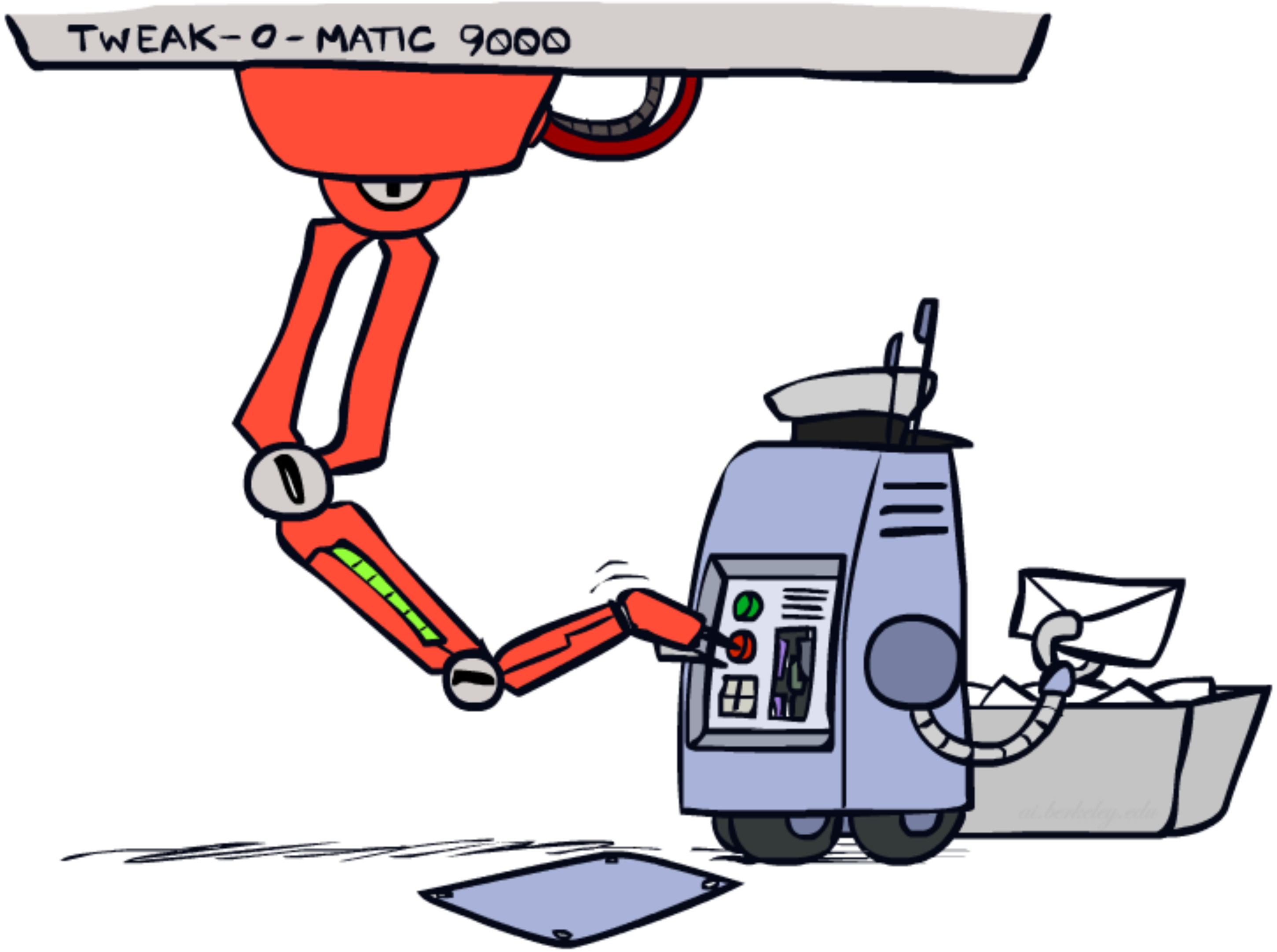
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

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



Do these make more sense?

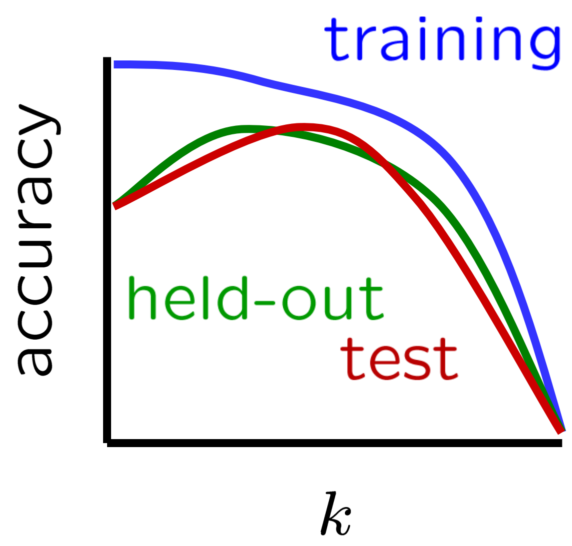
Tuning

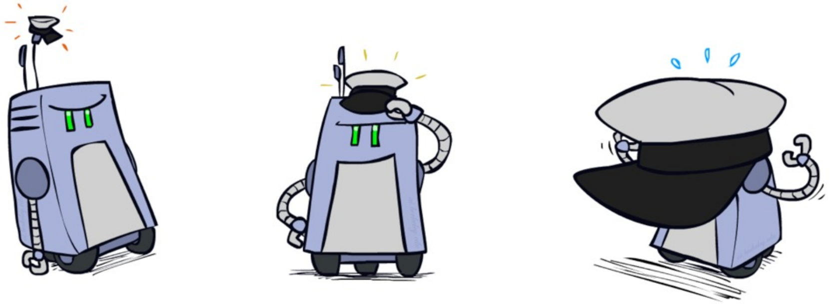


Tuning on Held-Out Data

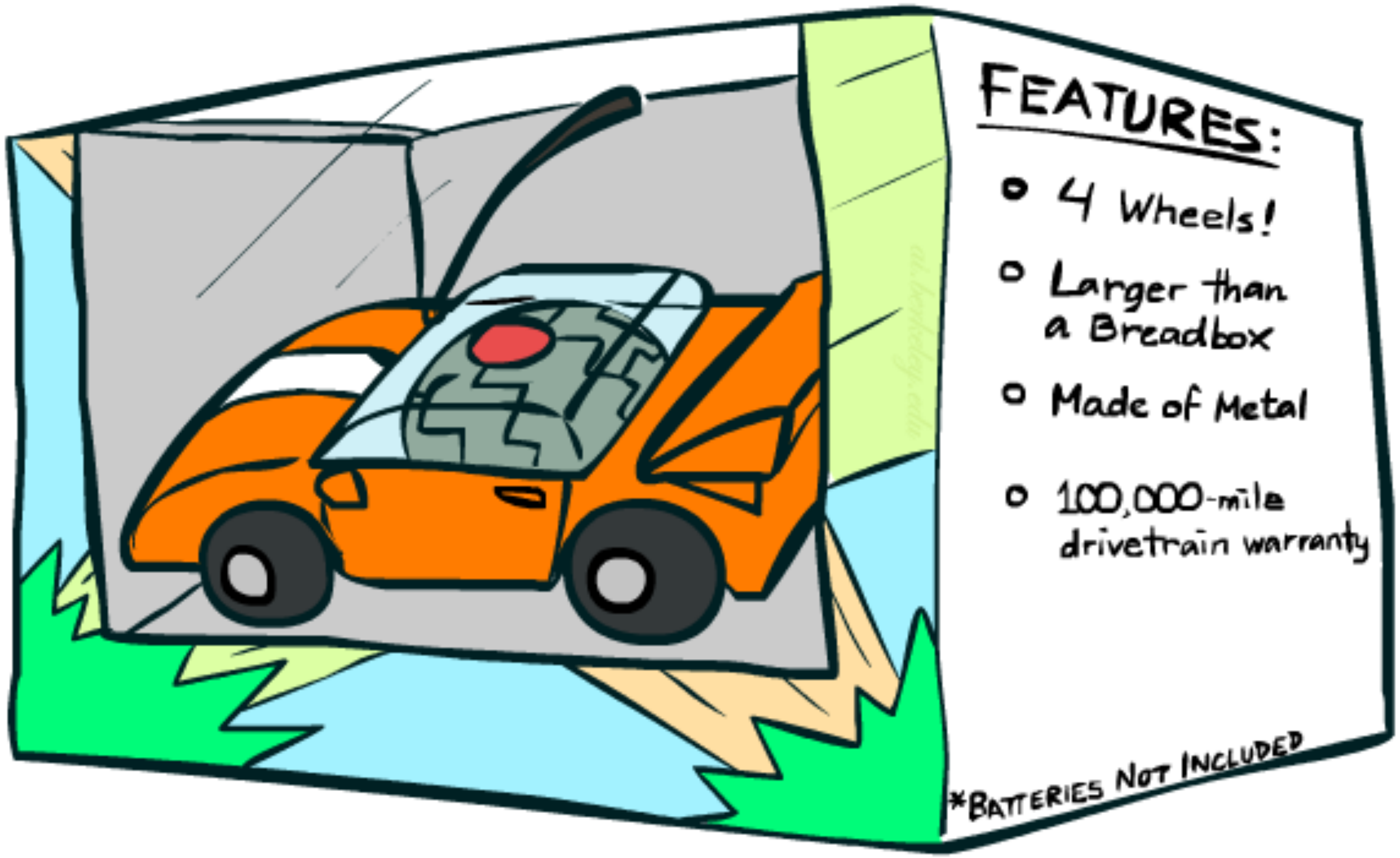
- Now we've got two kinds of unknowns
  - Parameters: the probabilities P(X|Y), P(Y)
  - Hyperparameters: e.g. the amount / type of smoothing to do, k, α

- 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 . . .
```

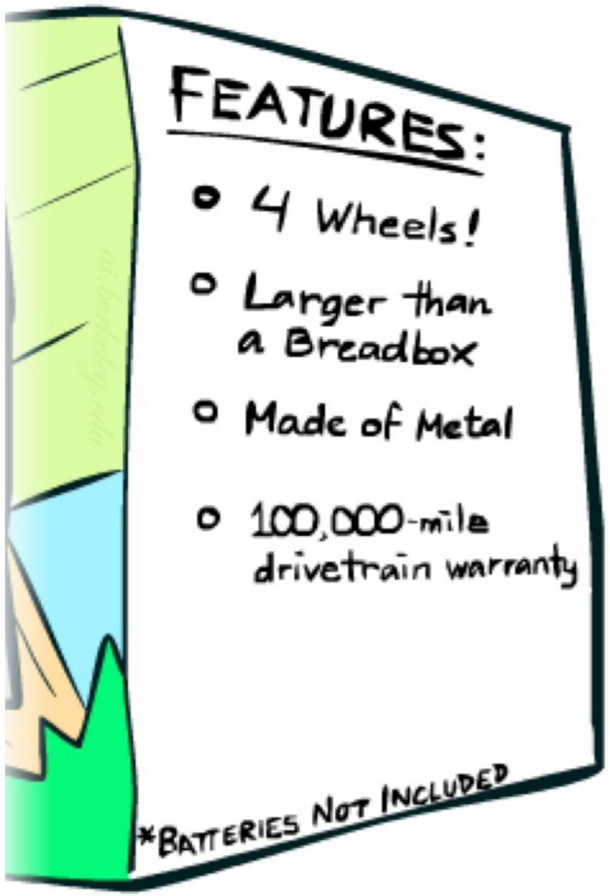
```
. . . To receive your $30 Amazon.com promotional certificate,
click through to

  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

- Next class we'll talk about classifiers which let you easily add arbitrary features more easily



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

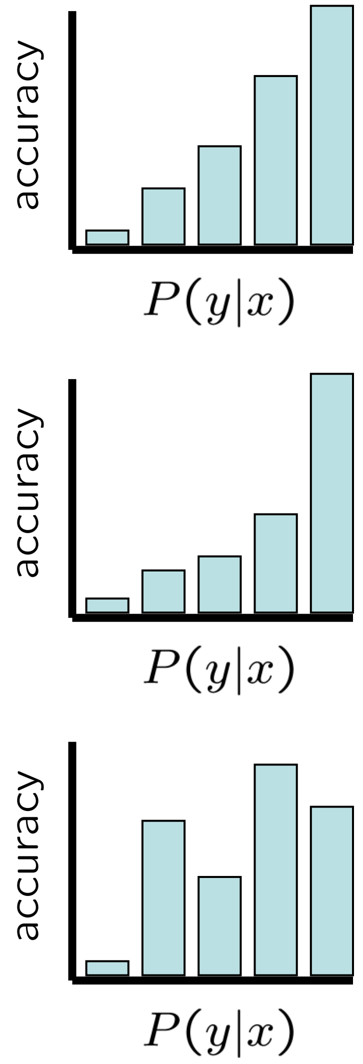
Confidences from a Classifier

- The confidence of a probabilistic classifier:
  - Posterior 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

Error-Driven Classification

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 . . .
```

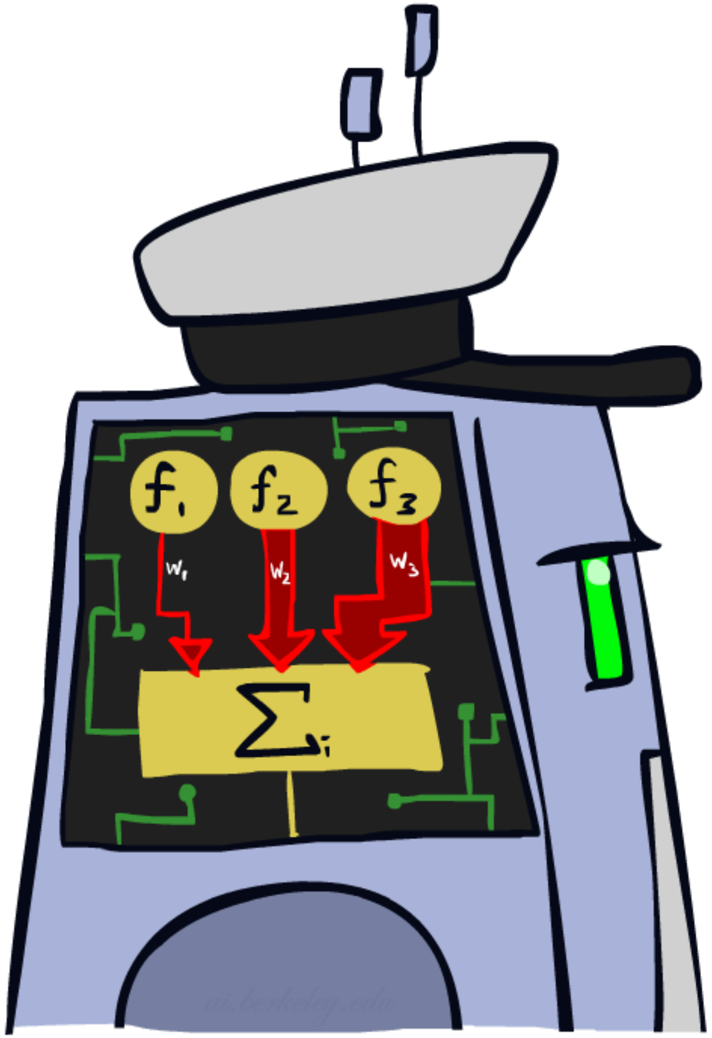
What to Do About Errors

- Problem: there's still spam in your inbox

- Need more features – words aren't enough!
  - Have you emailed the sender before?
  - Have 1M 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?

- Naïve Bayes models can incorporate a variety of features, but tend to do best in homogeneous cases (e.g. all features are word occurrences)

Linear Classifiers



Feature Vectors

x $\quad$ $f(x)$ $\quad$ 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
...
```

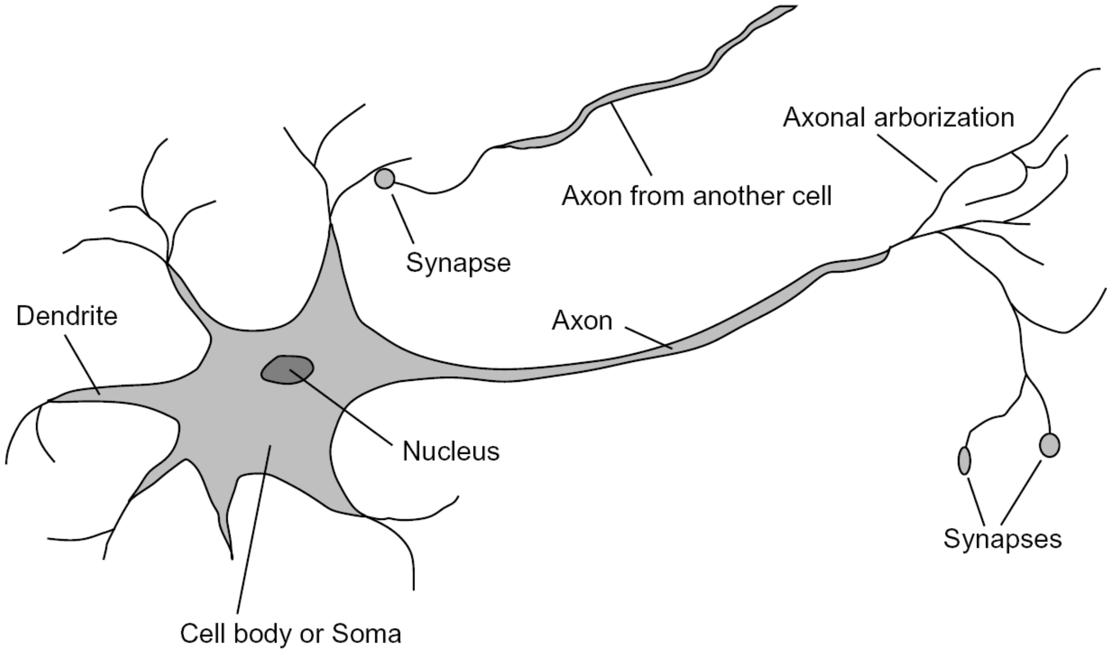
SPAM
or
+

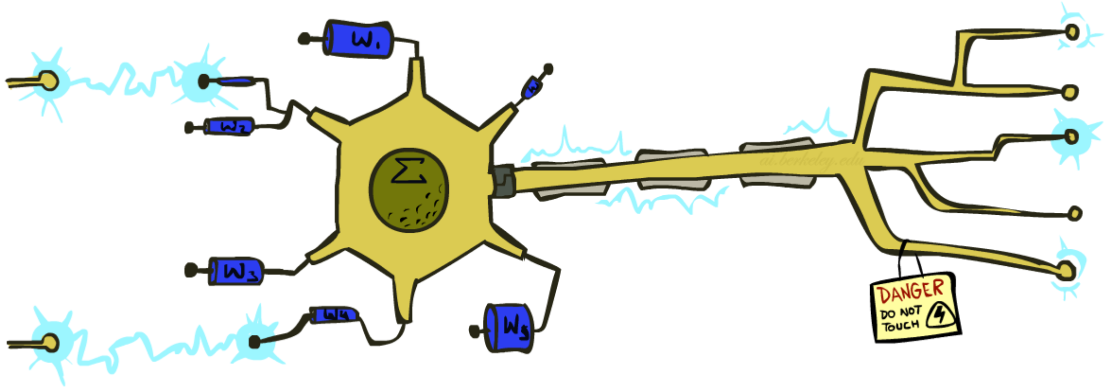
```
PIXEL-7,12   : 1
PIXEL-7,13   : 0
...
NUM_LOOPS    : 1
...
```

“2”

Some (Simplified) Biology

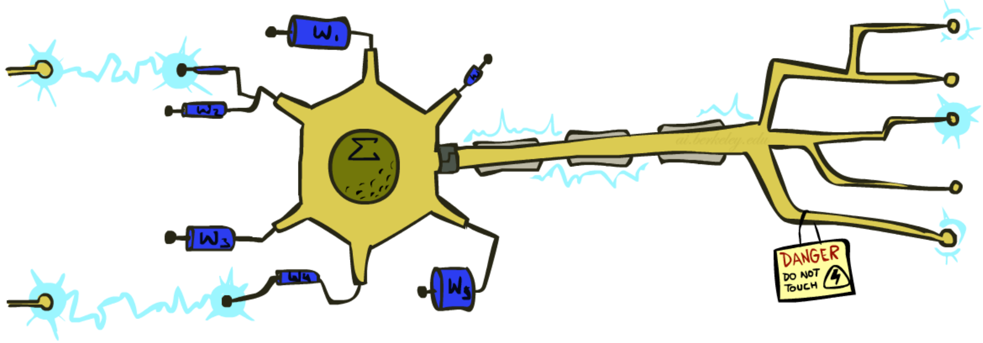
- Very loose inspiration: human neurons





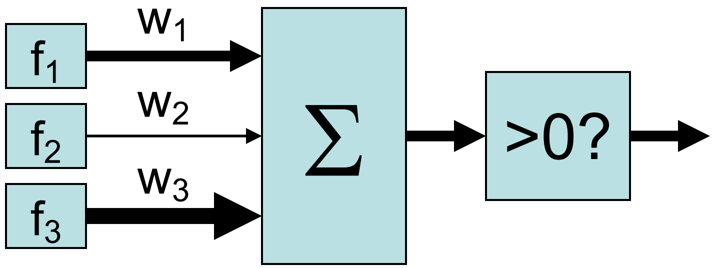
Linear Classifiers

- 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

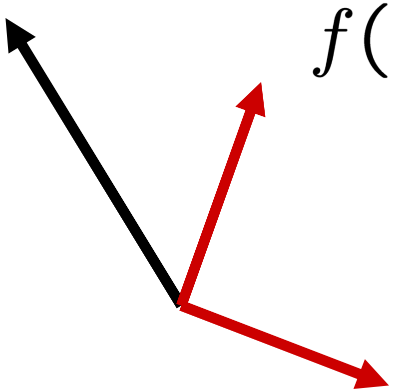


Weights

- 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
...
```

w



$f(x_1)$

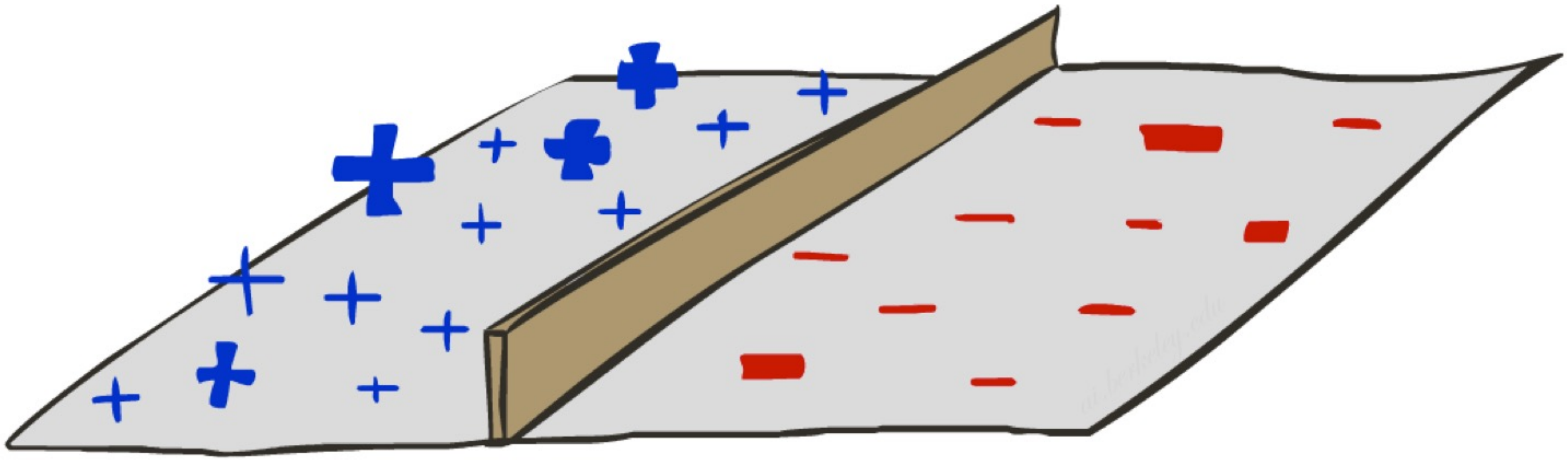
```
# free       : 2
YOUR_NAME    : 0
MISSPELLED   : 2
FROM_FRIEND  : 0
...
```

$f(x_2)$

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

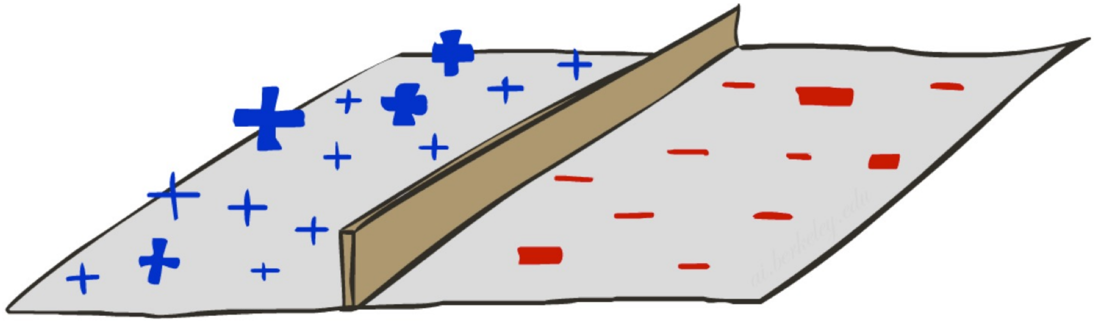
Dot product $w \cdot f$ *positive means the positive class*

Decision Rules



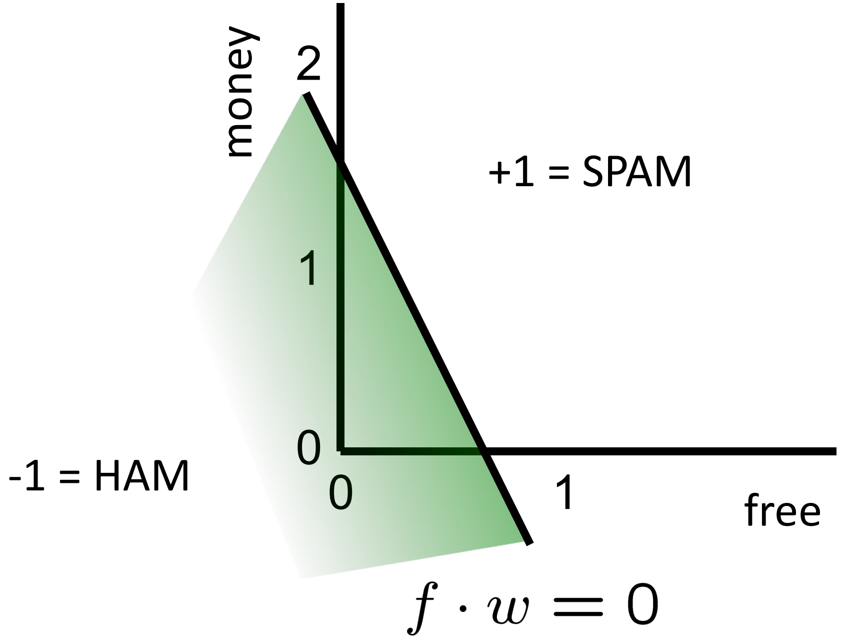
Binary Decision Rule

- 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



$$w$$

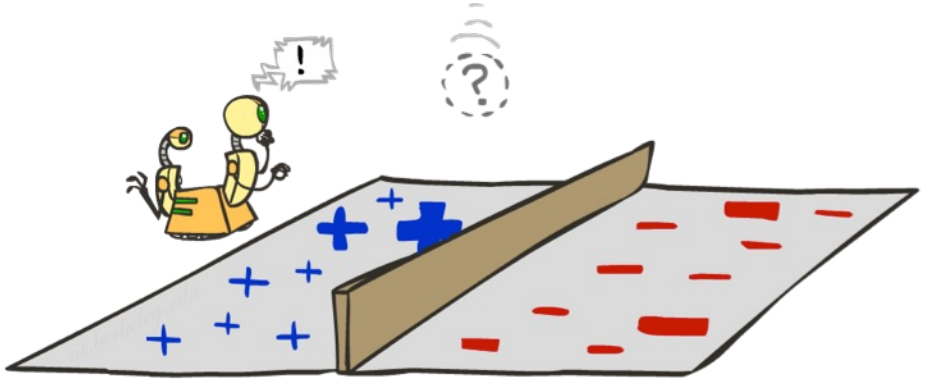
```
BIAS  : -3
free  :  4
money :  2
...
```



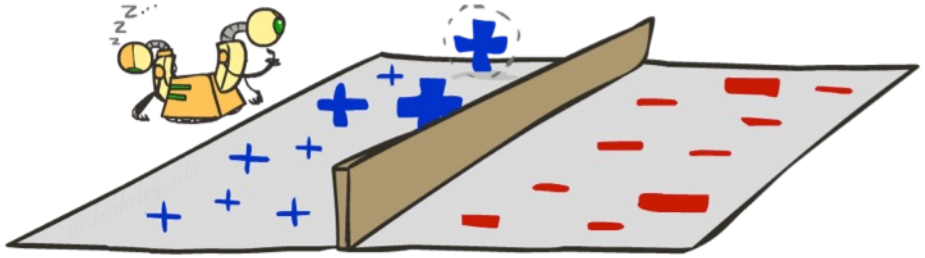
Weight Updates

Learning: Binary Perceptron

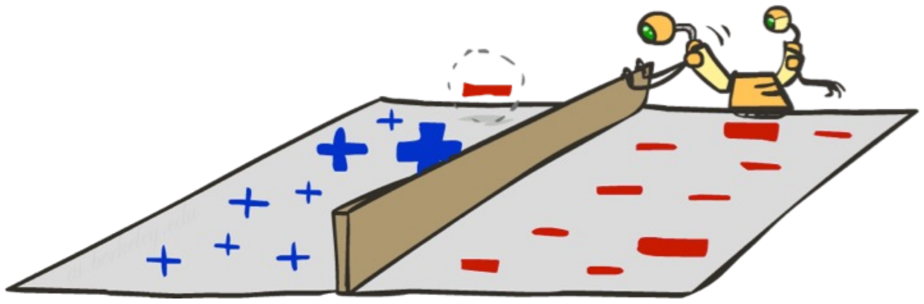
- Start with weights = 0
- For each training instance:
  - Classify with current weights



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



  - If wrong: adjust the weight vector



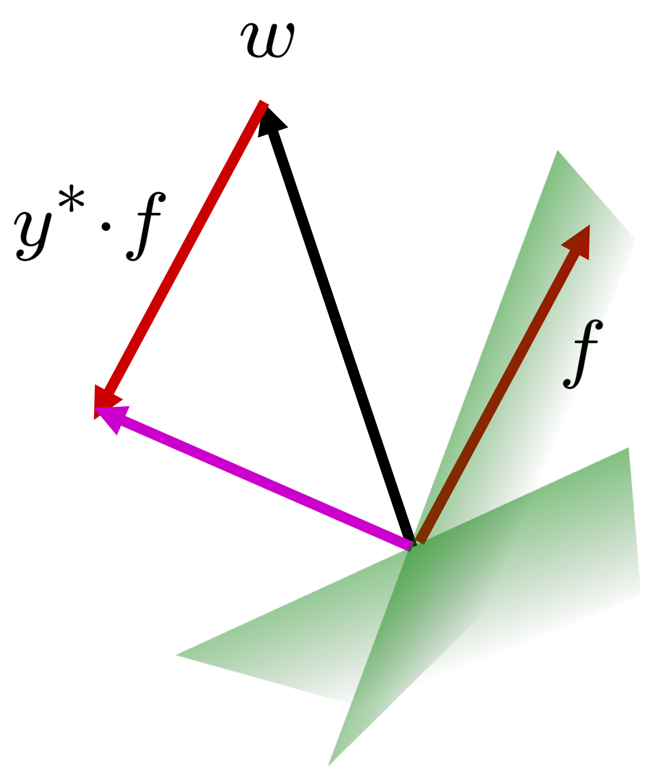
Learning: Binary Perceptron

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

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

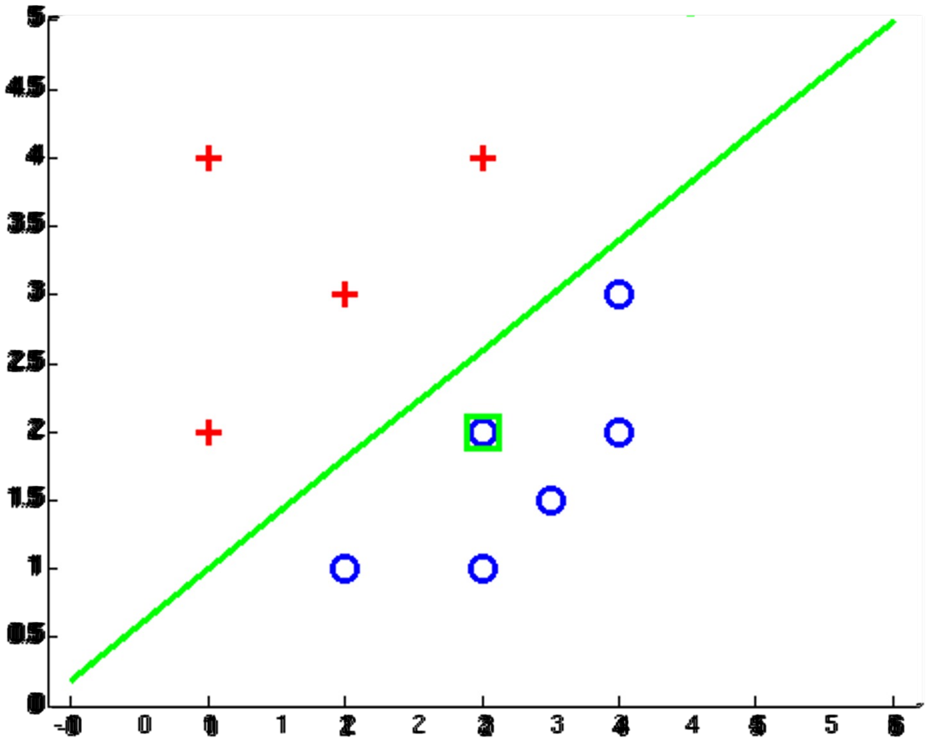
  - If correct (i.e., y=y*), no change!
  - If wrong: adjust the weight vector by adding or subtracting the feature vector. Subtract if y* is -1.

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



Examples: Perceptron

- Separable Case



Multiclass Decision Rule

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

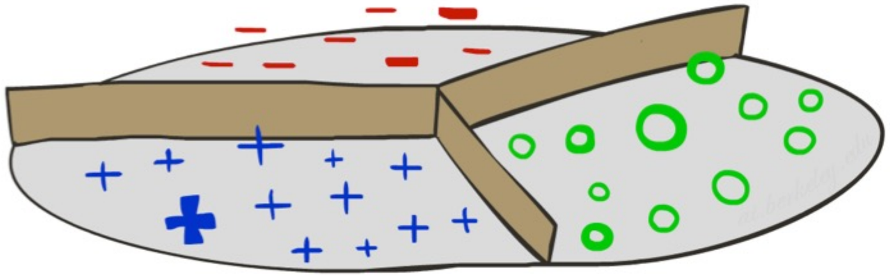
$$w_y$$

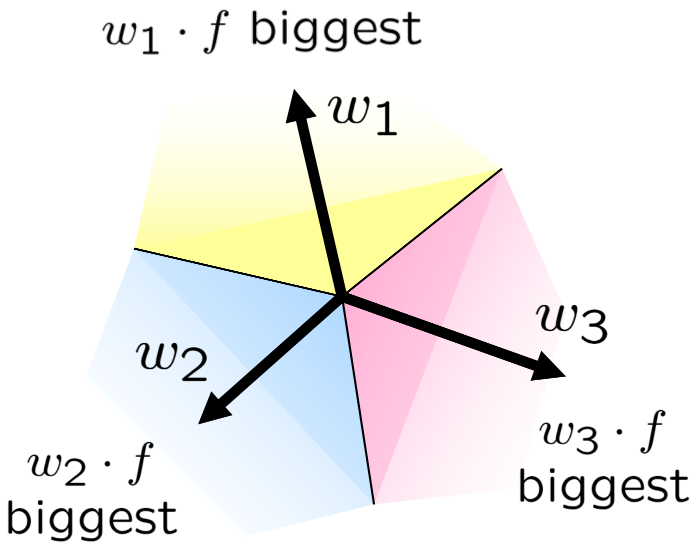
  - Score (activation) of a class y:

$$w_y \cdot f(x)$$

  - 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

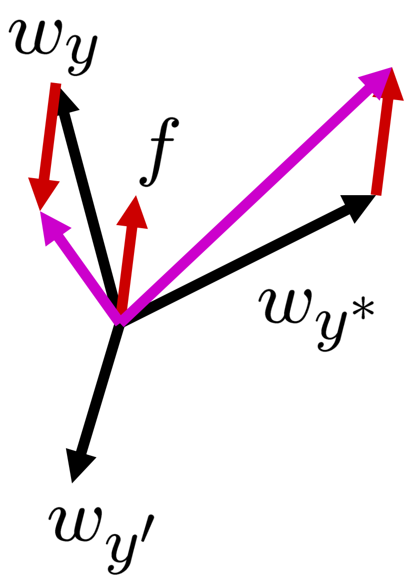
- Start with all weights = 0
- Pick up training examples one by one
- Predict with current weights

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

- 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

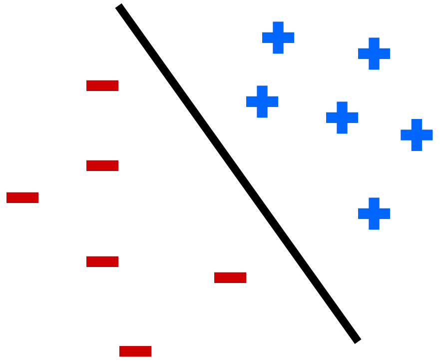
- Separability: true if some parameters get the training set perfectly correct

- Convergence: if the training is separable, perceptron will eventually converge (binary case)

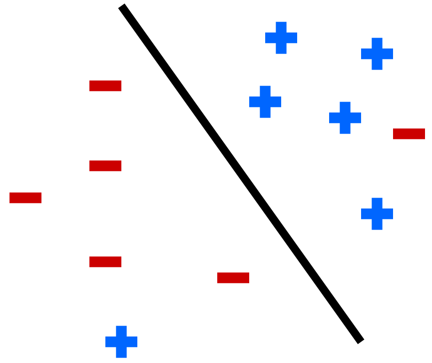
- Mistake Bound: the maximum number of mistakes (binary case) related to the *margin* or degree of separability

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

Separable

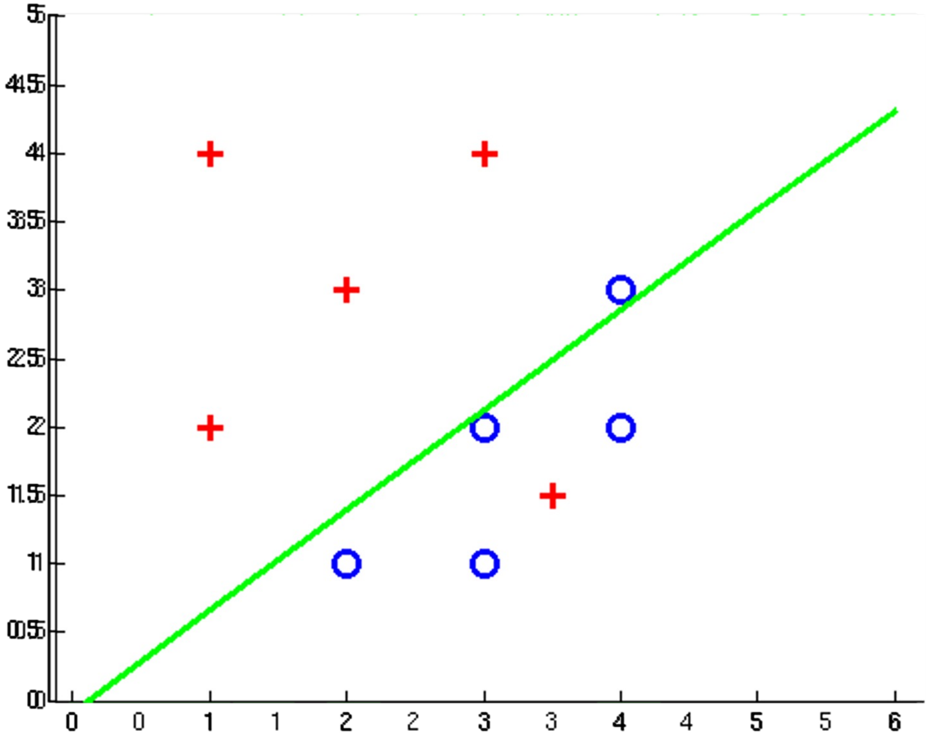


Non-Separable

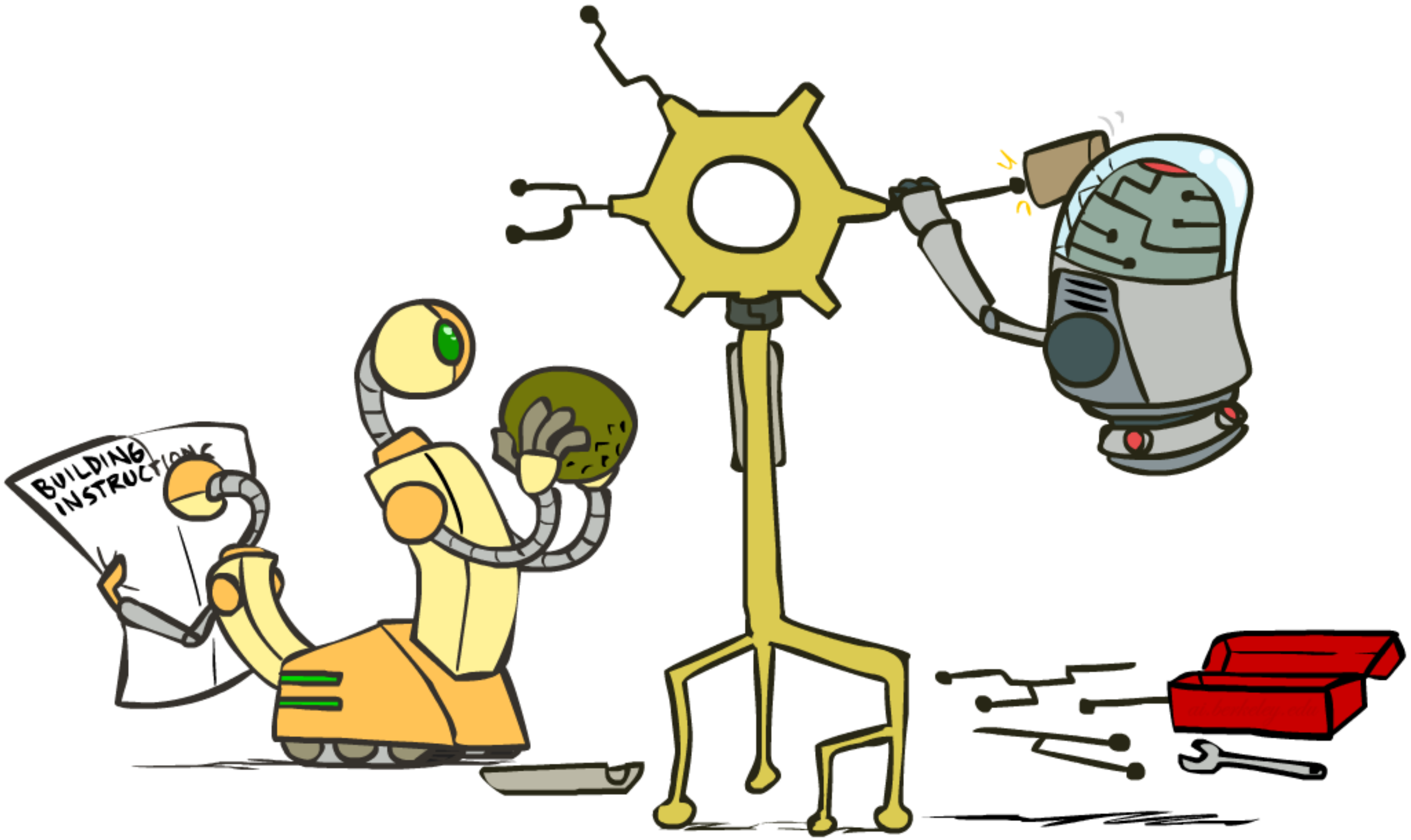


Examples: Perceptron

- Non-Separable Case

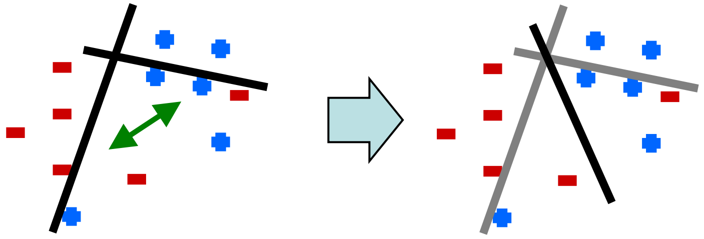


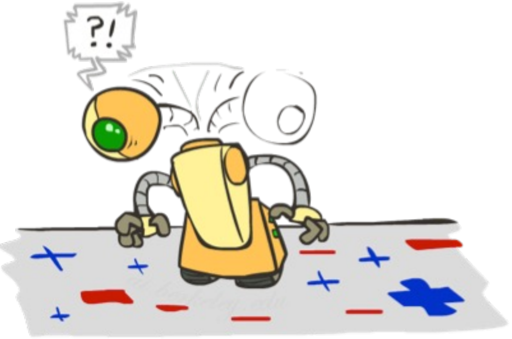
Improving the Perceptron



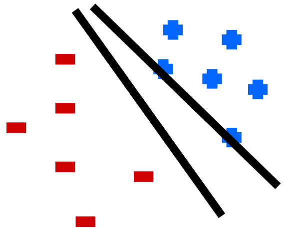
Problems with the Perceptron

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

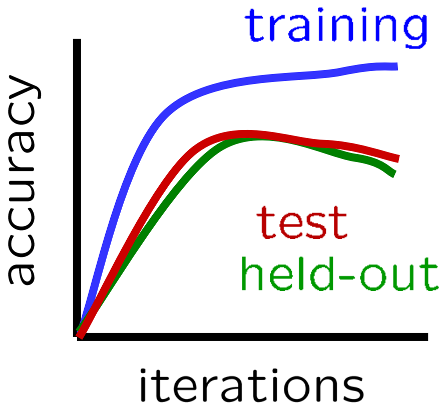


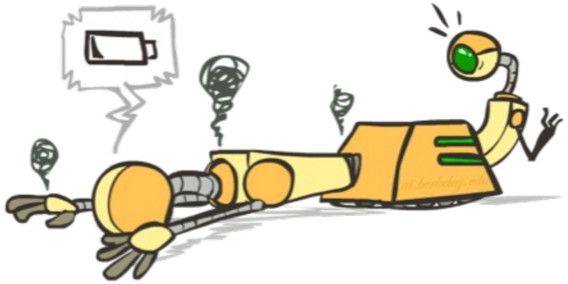


- Mediocre generalization: finds a “barely” separating solution



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





Fixing the Perceptron

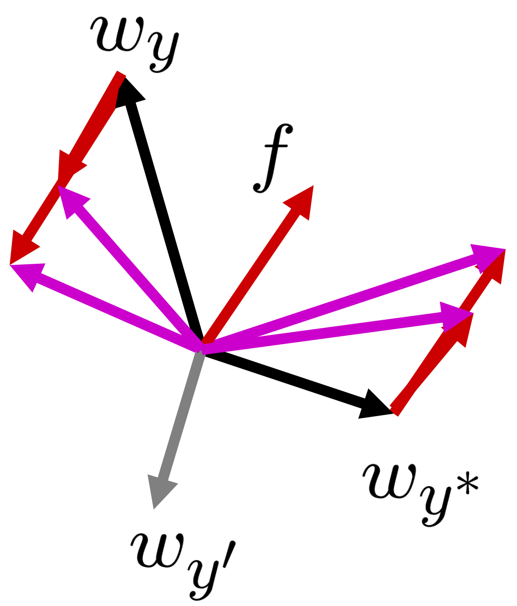
- Idea: adjust the weight update to mitigate these effects

- MIRA*: choose an update size that fixes the current mistake…
- … but, minimizes the change to w

$$\min_{w} \ \frac{1}{2} \sum_{y} ||w_y - w'_y||^2$$

$$w_{y^*} \cdot f(x) \geq w_y \cdot f(x) + 1$$

- The +1 helps to generalize



Guessed y instead of y^* on example x with features $f(x)$

$$w_y = w'_y - \tau f(x)$$
$$w_{y^*} = w'_{y^*} + \tau f(x)$$

* Margin Infused Relaxed Algorithm

Minimum Correcting Update

$$\min_{w} \; \frac{1}{2}\sum_{y} ||w_y - w'_y||^2$$

$$w_{y^*} \cdot f \geq w_y \cdot f + 1$$

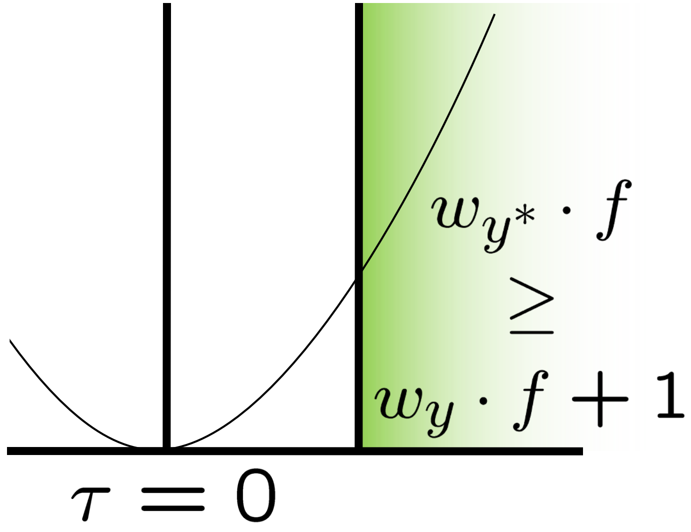
$$\min_{\tau} \; ||\tau f||^2$$

$$w_{y^*} \cdot f \geq w_y \cdot f + 1$$

$$(w'_{y^*} + \tau f) \cdot f = (w'_y - \tau f) \cdot f + 1$$

$$\tau = \frac{(w'_y - w'_{y^*}) \cdot f + 1}{2 f \cdot f}$$

$$\boxed{\begin{aligned} w_y &= w'_y - \tau f(x) \\ w_{y^*} &= w'_{y^*} + \tau f(x) \end{aligned}}$$

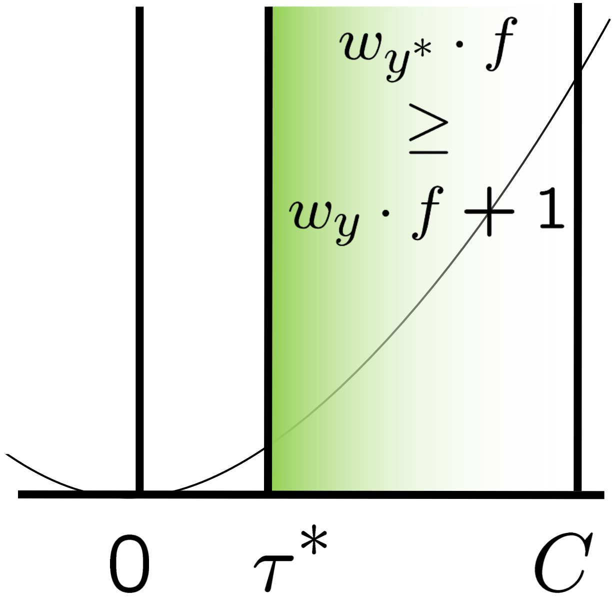


min not τ=0, or would not have made an error, so min will be where equality holds

Maximum Step Size

- In practice, it's also bad to make updates that are too large
  - Example may be labeled incorrectly
  - You may not have enough features
  - Solution: cap the maximum possible value of τ with some constant C

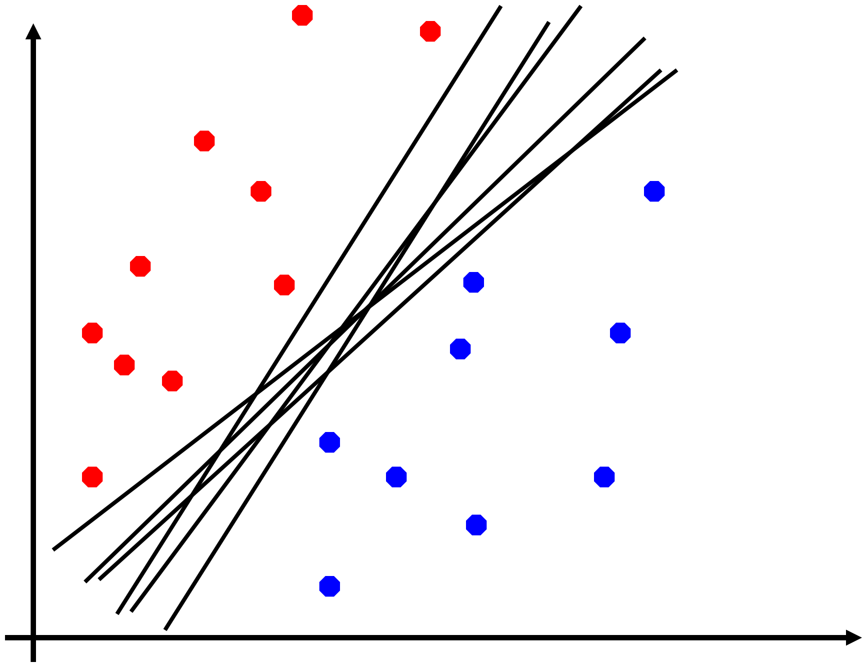
$$\tau^* = \min\left(\frac{(w'_y - w'_{y^*}) \cdot f + 1}{2f \cdot f}, C\right)$$



  - Corresponds to an optimization that assumes non-separable data
  - Usually converges faster than perceptron
  - Usually better, especially on noisy data

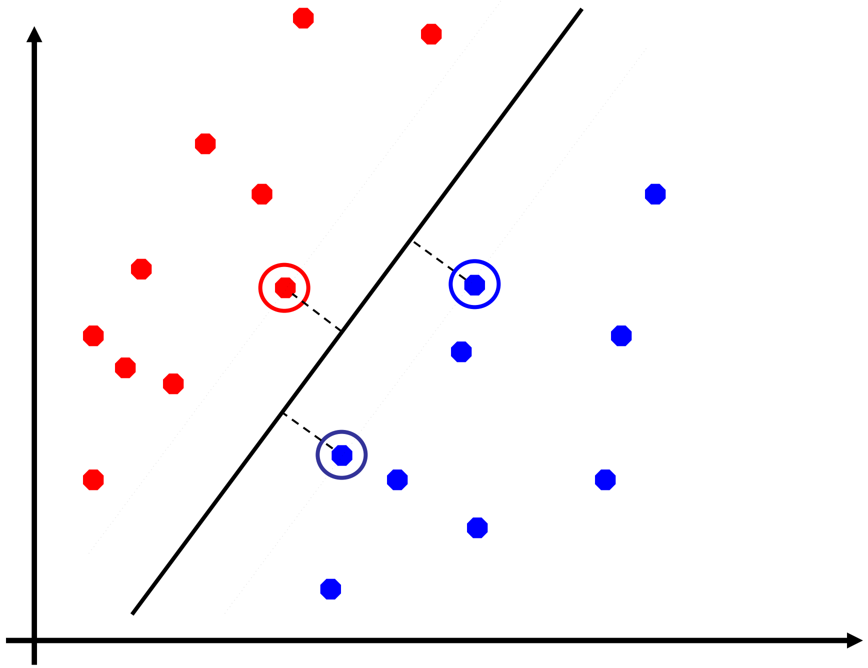
Linear Separators

- Which of these linear separators is optimal?



Support Vector Machines

- Maximizing the margin: good according to intuition, theory, practice
- Only support vectors matter; other training examples are ignorable
- Support vector machines (SVMs) find the separator with max margin
- Basically, SVMs are MIRA where you optimize over all examples at once



MIRA

$$\min_w \frac{1}{2}||w - w'||^2$$

$$w_{y^*} \cdot f(x_i) \geq w_y \cdot f(x_i) + 1$$

SVM

$$\min_w \frac{1}{2}||w||^2$$

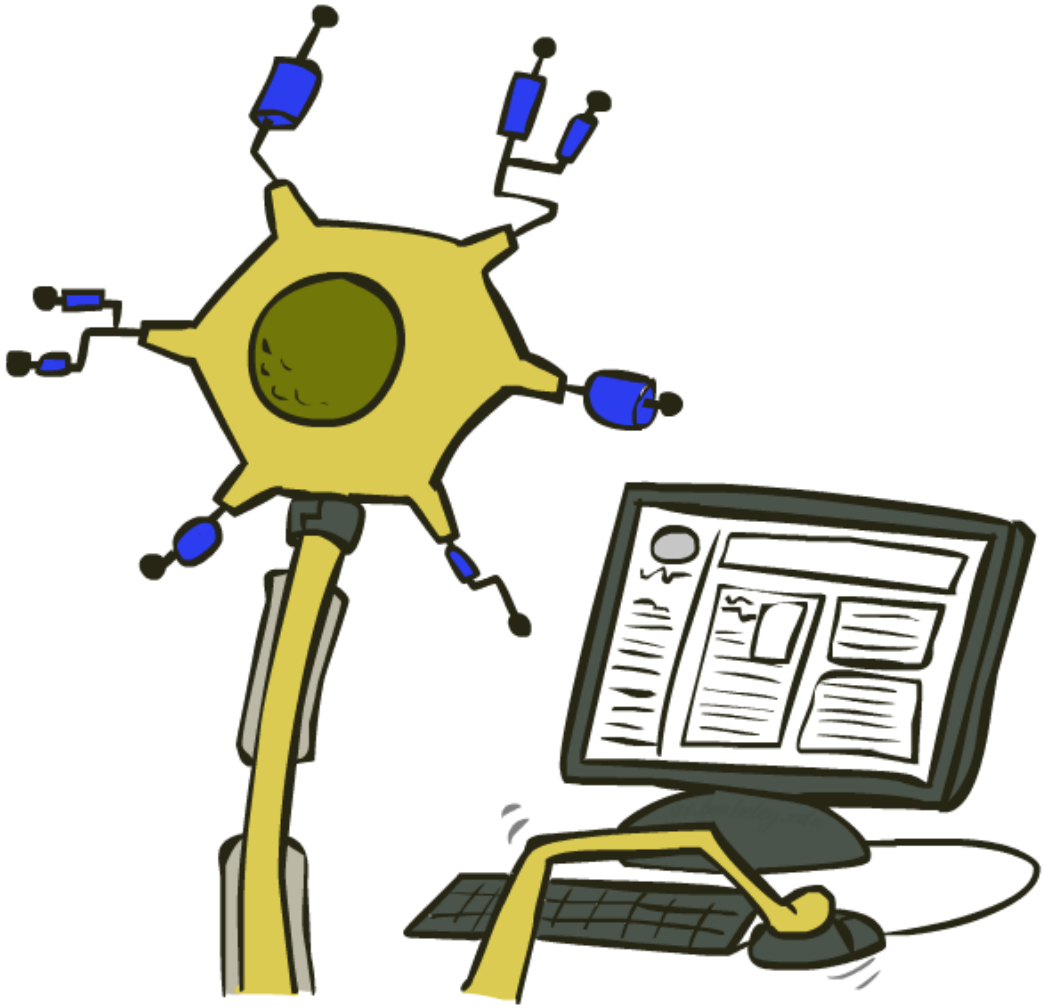
$$\forall i, y \; w_{y^*} \cdot f(x_i) \geq w_y \cdot f(x_i) + 1$$

Classification: Comparison

- Naïve Bayes
  - Builds a model training data
  - Gives prediction probabilities
  - Strong assumptions about feature independence
  - One pass through data (counting)

- Perceptrons / MIRA:
  - Makes less assumptions about data
  - Mistake-driven learning
  - Multiple passes through data (prediction)
  - Often more accurate

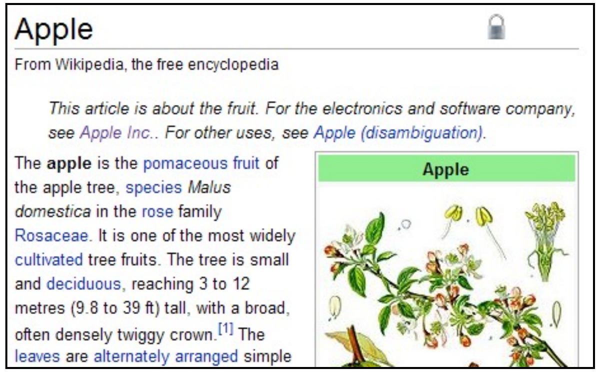
Web Search



Extension: Web Search

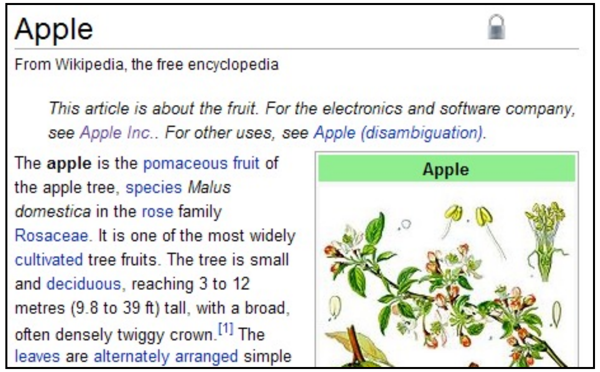
- Information retrieval:
  - Given information needs, produce information
  - Includes, e.g. web search, question answering, and classic IR
- Web search: not exactly classification, but rather ranking

x = “Apple Computers”



Feature-Based Ranking

x = “Apple Computer”

$f(x,$ 

$) = [0.3\ 5\ 0\ 0\ \ldots]$

$f(x,$ 

$) = [0.8\ 4\ 2\ 1\ \ldots]$

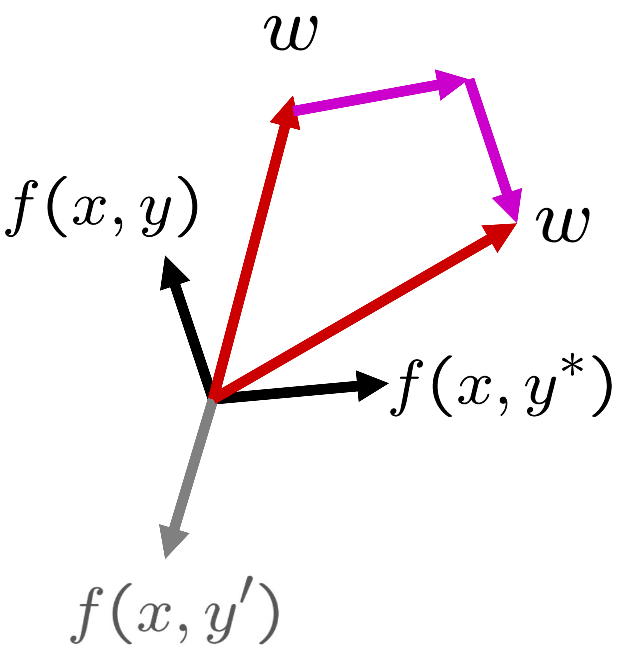
Perceptron for Ranking

- Inputs x
- Candidates y
- Many feature vectors: $f(x, y)$
- One weight vector: w
  - Prediction:

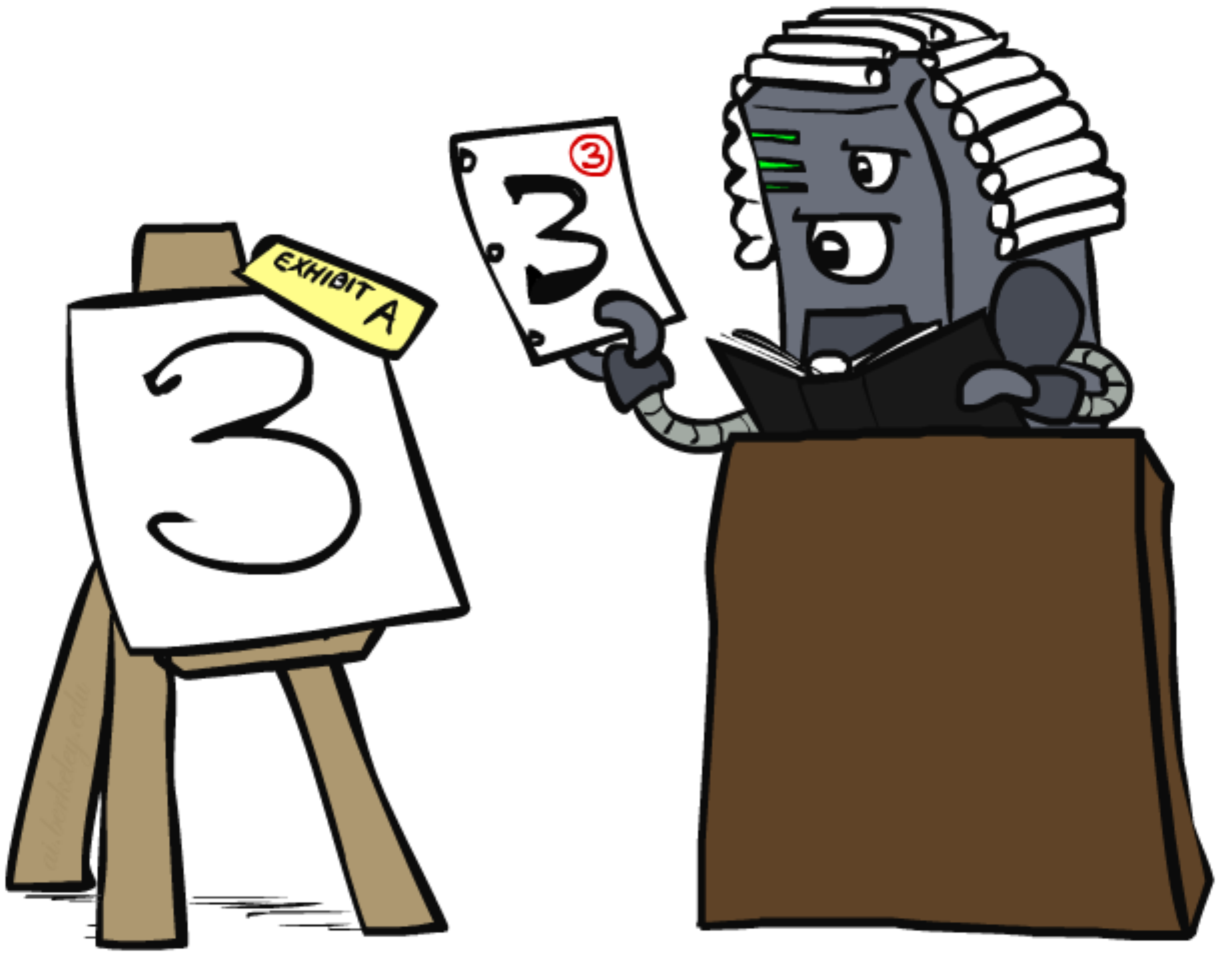
    $$y = \arg\max_y \; w \cdot f(x, y)$$

  - Update (if wrong):

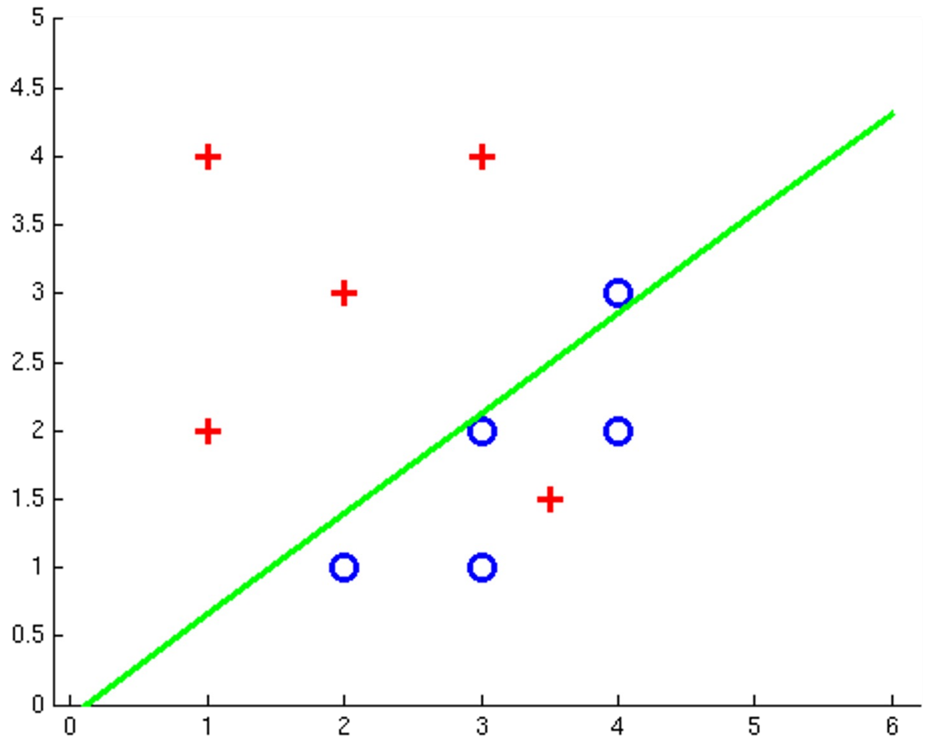
    $$w = w + f(x, y^*) - f(x, y)$$



Case-Based Learning

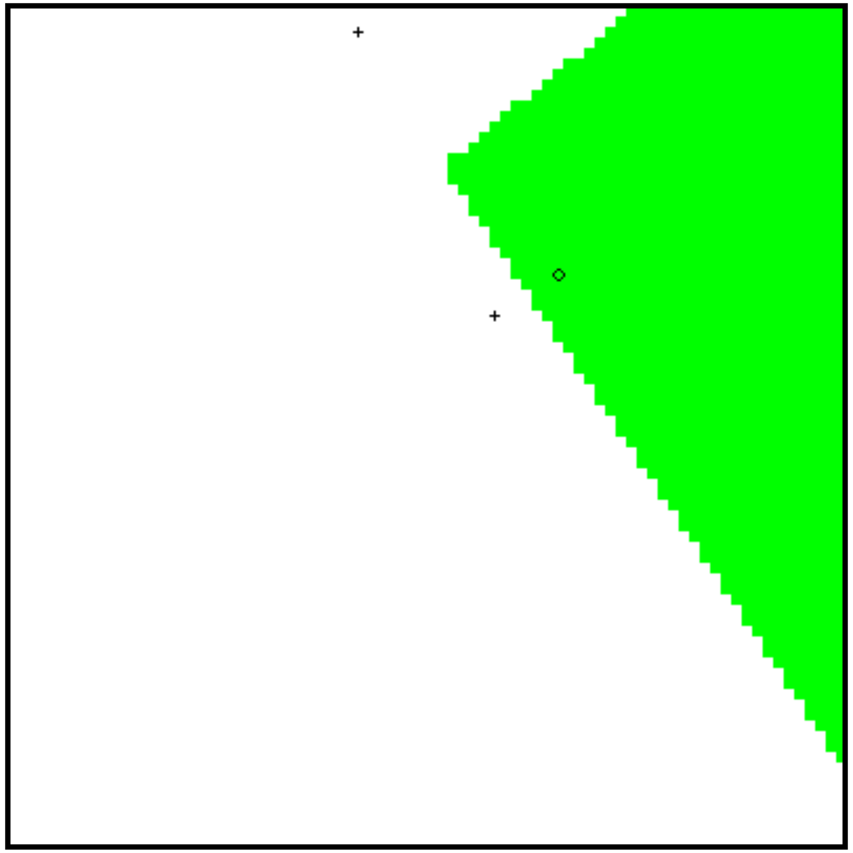


Non-Separable Data



Case-Based Reasoning

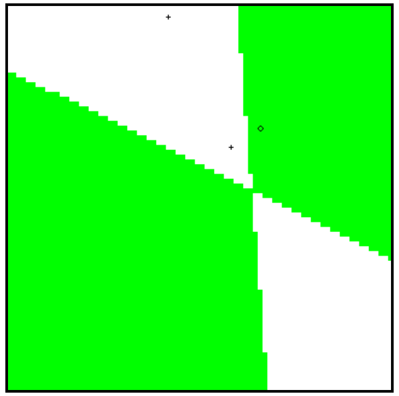
- Classification from similarity
  - Case-based reasoning
  - Predict an instance's label using similar instances
- Nearest-neighbor classification
  - 1-NN: copy the label of the most similar data point
  - K-NN: vote the k nearest neighbors (need a weighting scheme)
  - Key issue: how to define similarity
  - Trade-offs: Small k gives relevant neighbors, Large k gives smoother functions



http://www.cs.cmu.edu/~zhuxj/courseproject/knndemo/KNN.html

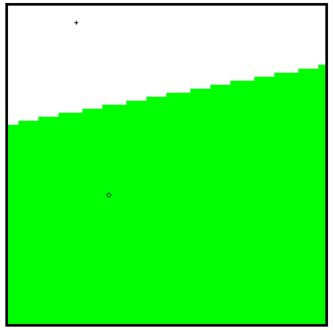
Parametric / Non-Parametric

- Parametric models:
  - Fixed set of parameters
  - More data means better settings
- Non-parametric models:
  - Complexity of the classifier increases with data
  - Better in the limit, often worse in the non-limit
- (K)NN is non-parametric

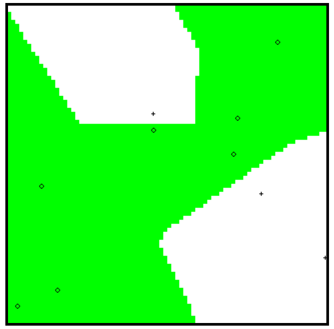


Truth

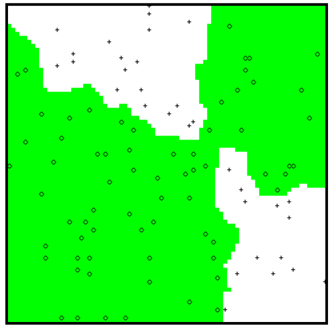
2 Examples



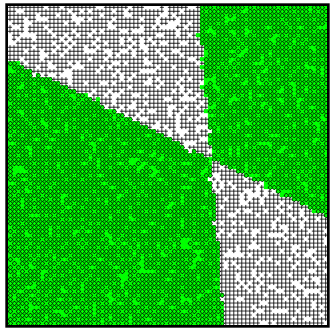
10 Examples



100 Examples

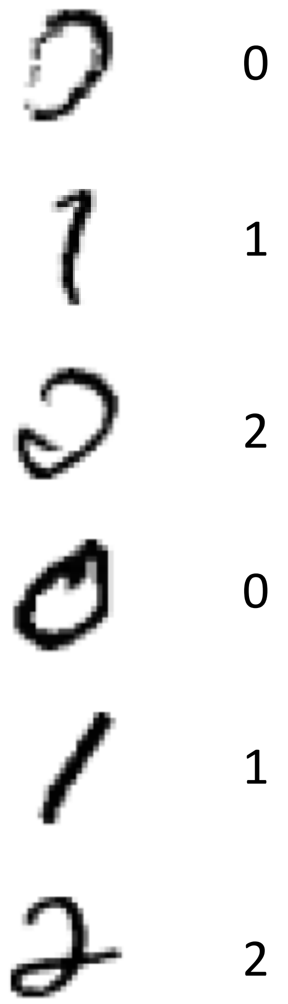


10000 Examples



Nearest-Neighbor Classification

- Nearest neighbor for digits:
  - Take new image
  - Compare to all training images
  - Assign based on closest example



- Encoding: image is vector of intensities:

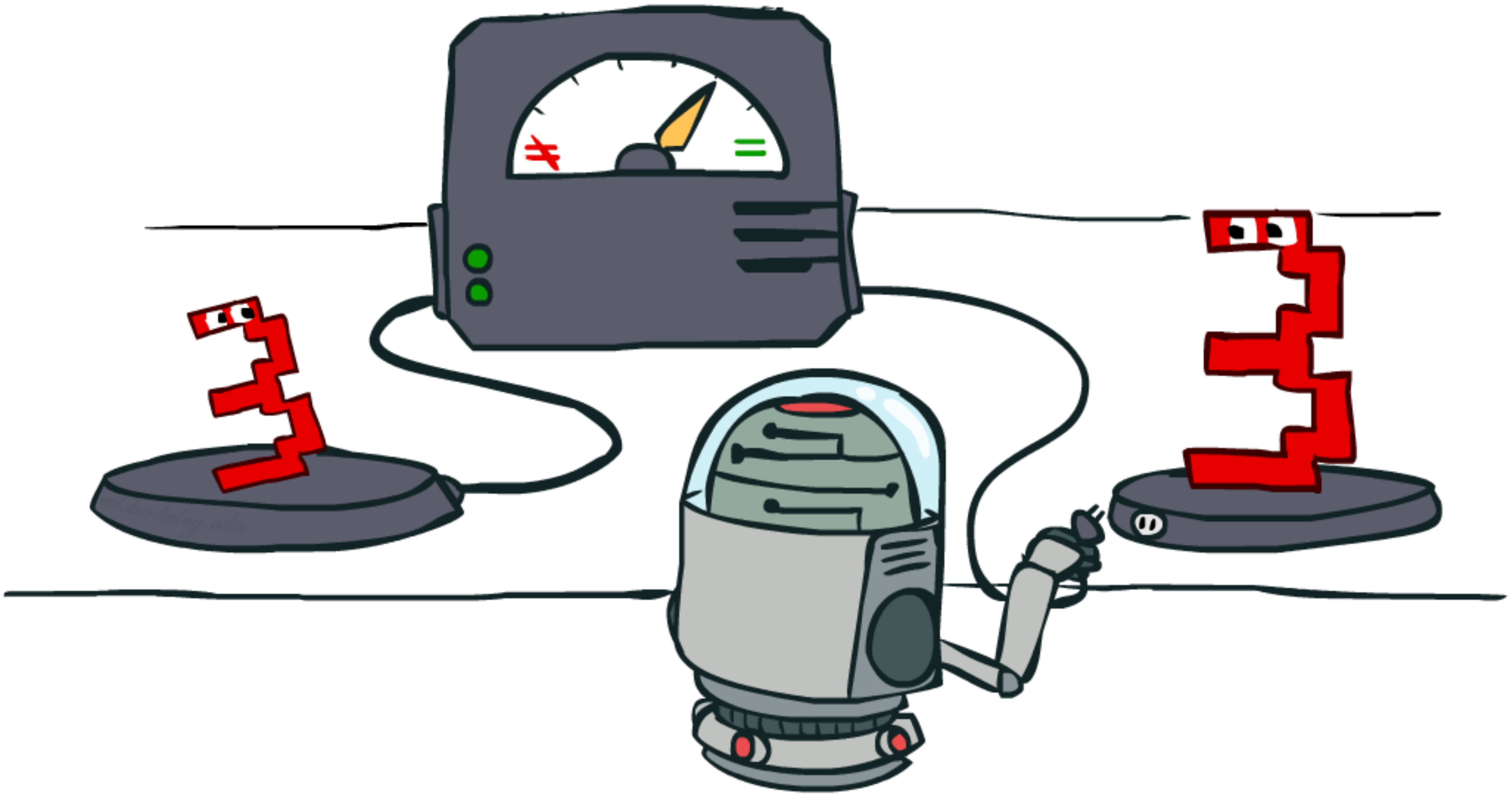
$$= \langle 0.0\ \ 0.0\ \ 0.3\ \ 0.8\ \ 0.7\ \ 0.1 \ldots 0.0 \rangle$$

- What's the similarity function?
  - Dot product of two images vectors?

$$\text{sim}(x, x') = x \cdot x' = \sum_i x_i x'_i$$

  - Usually normalize vectors so ||x|| = 1
  - min = 0 (when?), max = 1 (when?)

Similarity Functions



Basic Similarity

- Many similarities based on feature dot products:

$$\text{sim}(x, x') = f(x) \cdot f(x') = \sum_i f_i(x) f_i(x')$$

- If features are just the pixels:

$$\text{sim}(x, x') = x \cdot x' = \sum_i x_i x'_i$$

- Note: not all similarities are of this form

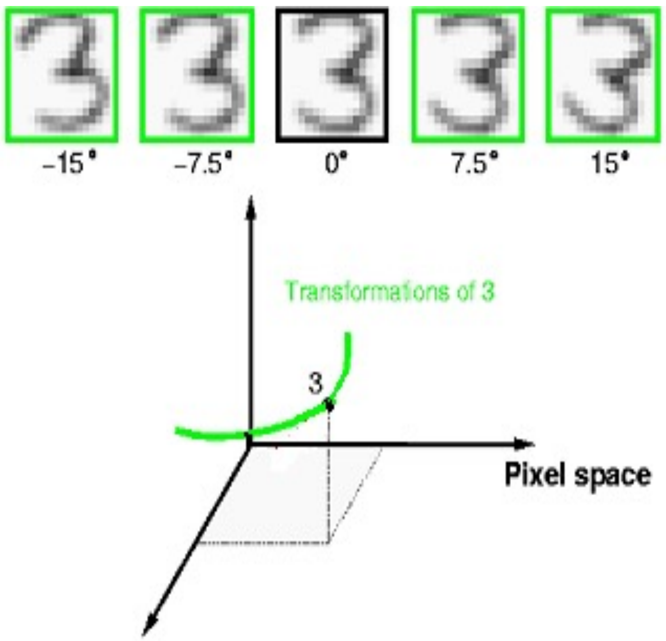
Invariant Metrics

- Better similarity functions use knowledge about vision
- Example: invariant metrics:
  - Similarities are invariant under certain transformations
  - Rotation, scaling, translation, stroke-thickness…
  - E.g:

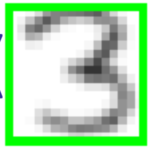
    - 16 x 16 = 256 pixels; a point in 256-dim space
    - These points have small similarity in R^{256} (why?)
  - How can we incorporate such invariances into our similarities?

This and next few slides adapted from Xiao Hu, UIUC

Rotation Invariant Metrics



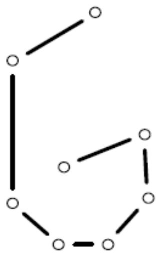
- Each example is now a curve in R^{256}
- Rotation invariant similarity:

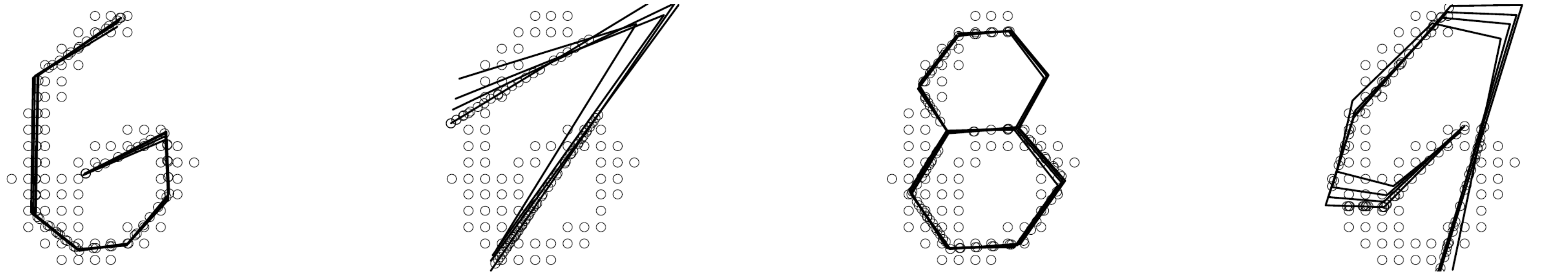
s'=max s(r(), r())

- E.g. highest similarity between images' rotation lines

Template Deformation

- Deformable templates:
  - An “ideal” version of each category
  - Best-fit to image using min variance
  - Cost for high distortion of template
  - Cost for image points being far from distorted template
- Used in many commercial digit recognizers





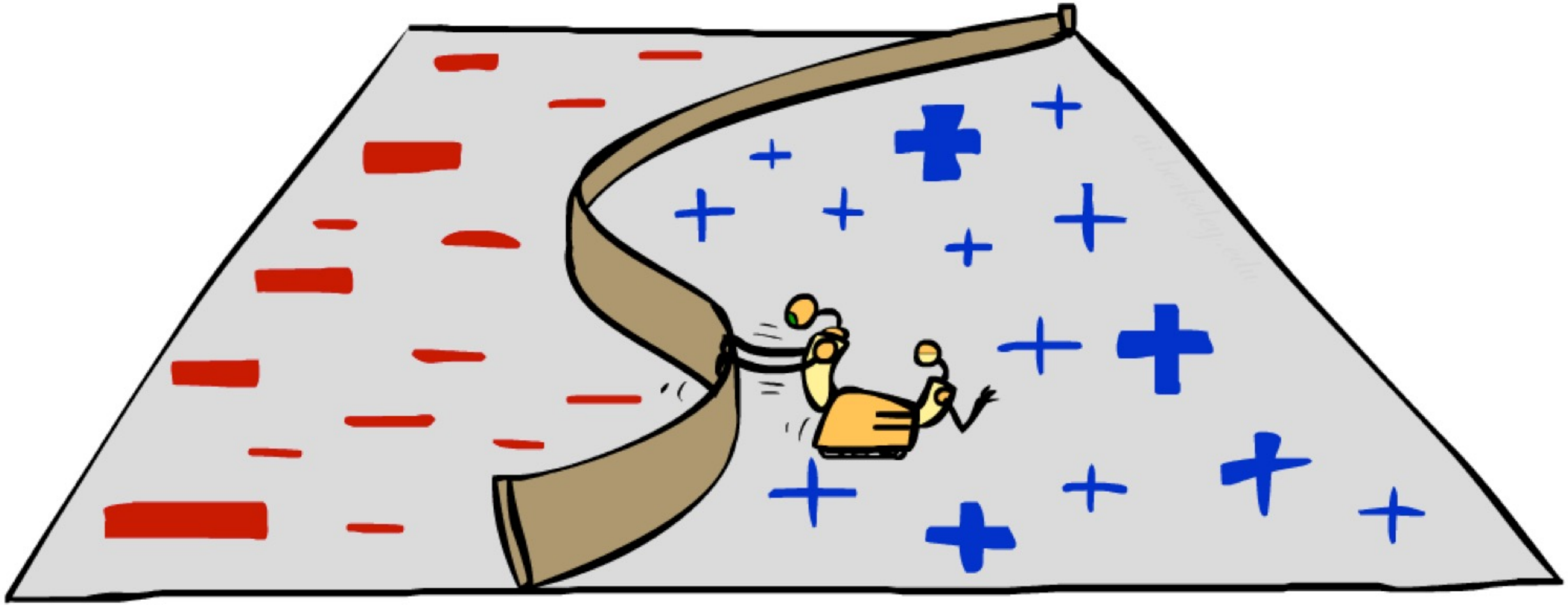
Examples from [Hastie 94]

A Tale of Two Approaches…

- Nearest neighbor-like approaches
  - Can use fancy similarity functions
  - Don’t actually get to do explicit learning

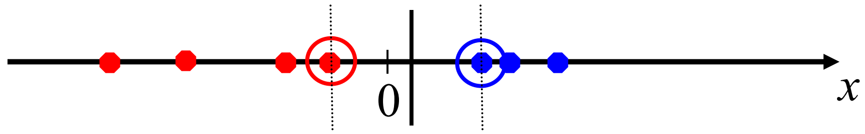
- Perceptron-like approaches
  - Explicit training to reduce empirical error
  - Can’t use fancy similarity, only linear
  - Or can they? Let’s find out!

Non-Linearity

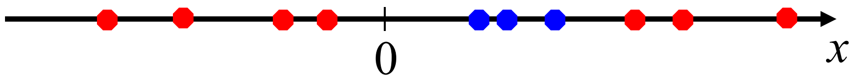


Non-Linear Separators

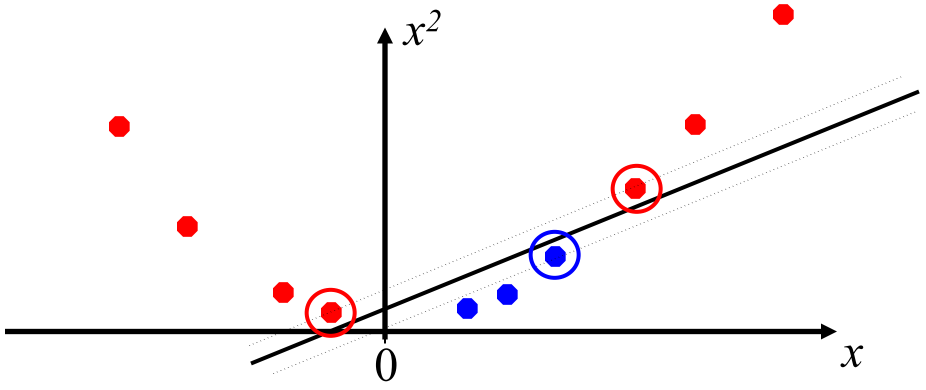
- Data that is linearly separable works out great for linear decision rules:



- But what are we going to do if the dataset is just too hard?



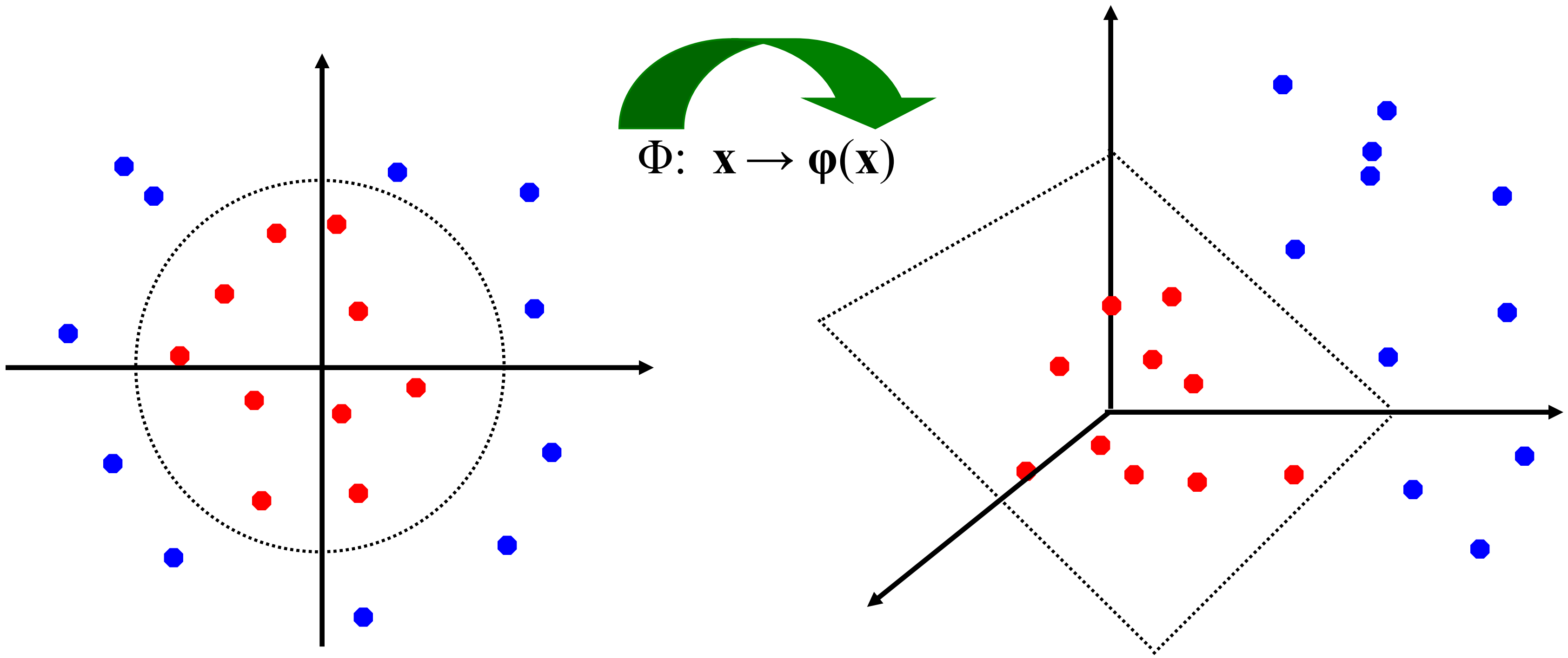
- How about… mapping data to a higher-dimensional space:



This and next few slides adapted from Ray Mooney, UT

Non-Linear Separators

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



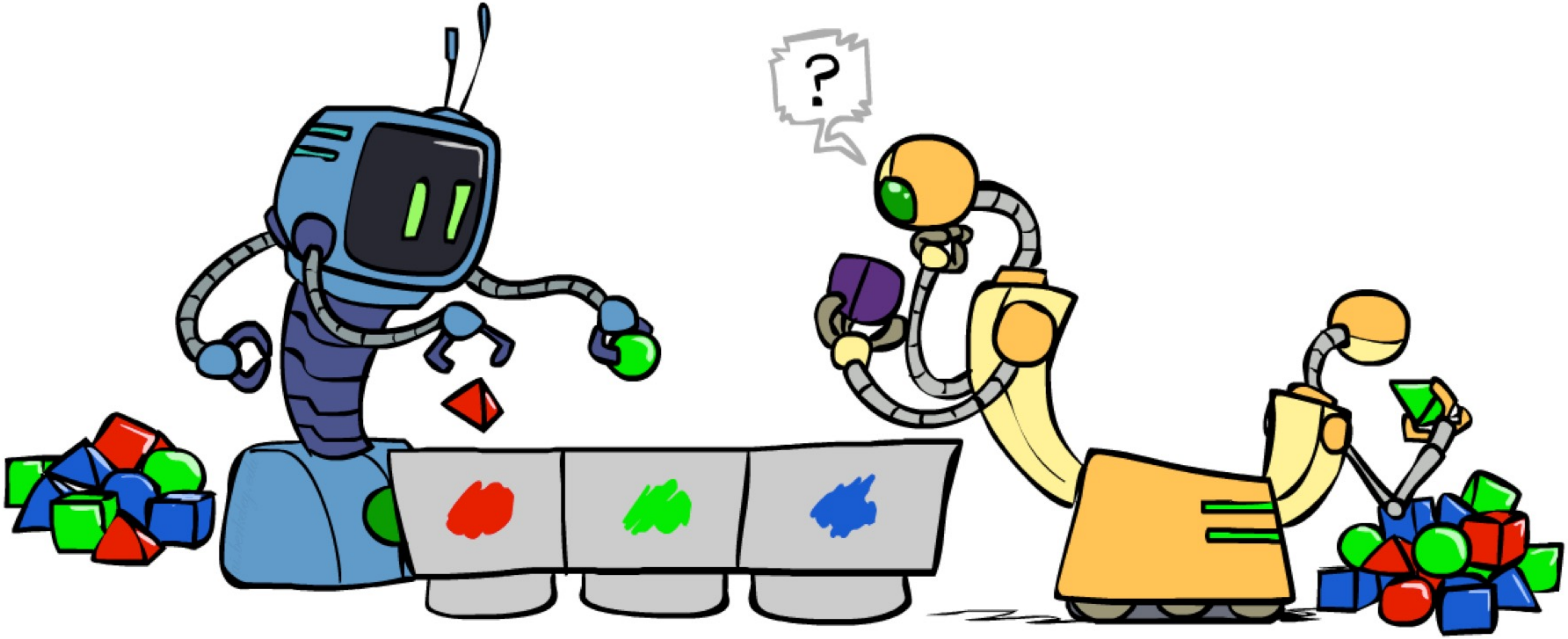
Recap: Classification

- Classification systems:
  - Supervised learning
  - Make a prediction given evidence
  - We've seen several methods for this
  - Useful when you have labeled data

Clustering

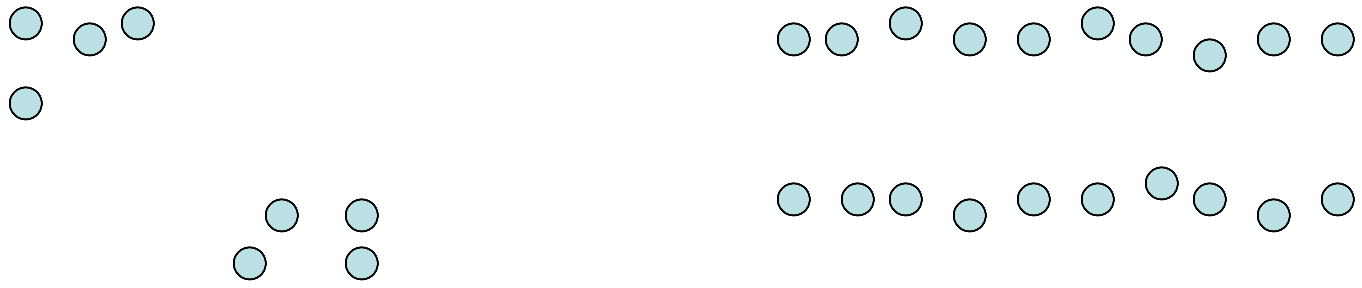
- Clustering systems:
  - Unsupervised learning
  - Detect patterns in unlabeled data
    - E.g. group emails or search results
    - E.g. find categories of customers
    - E.g. detect anomalous program executions
  - Useful when don't know what you're looking for
  - Requires data, but no labels
  - Often get gibberish

Clustering



Clustering

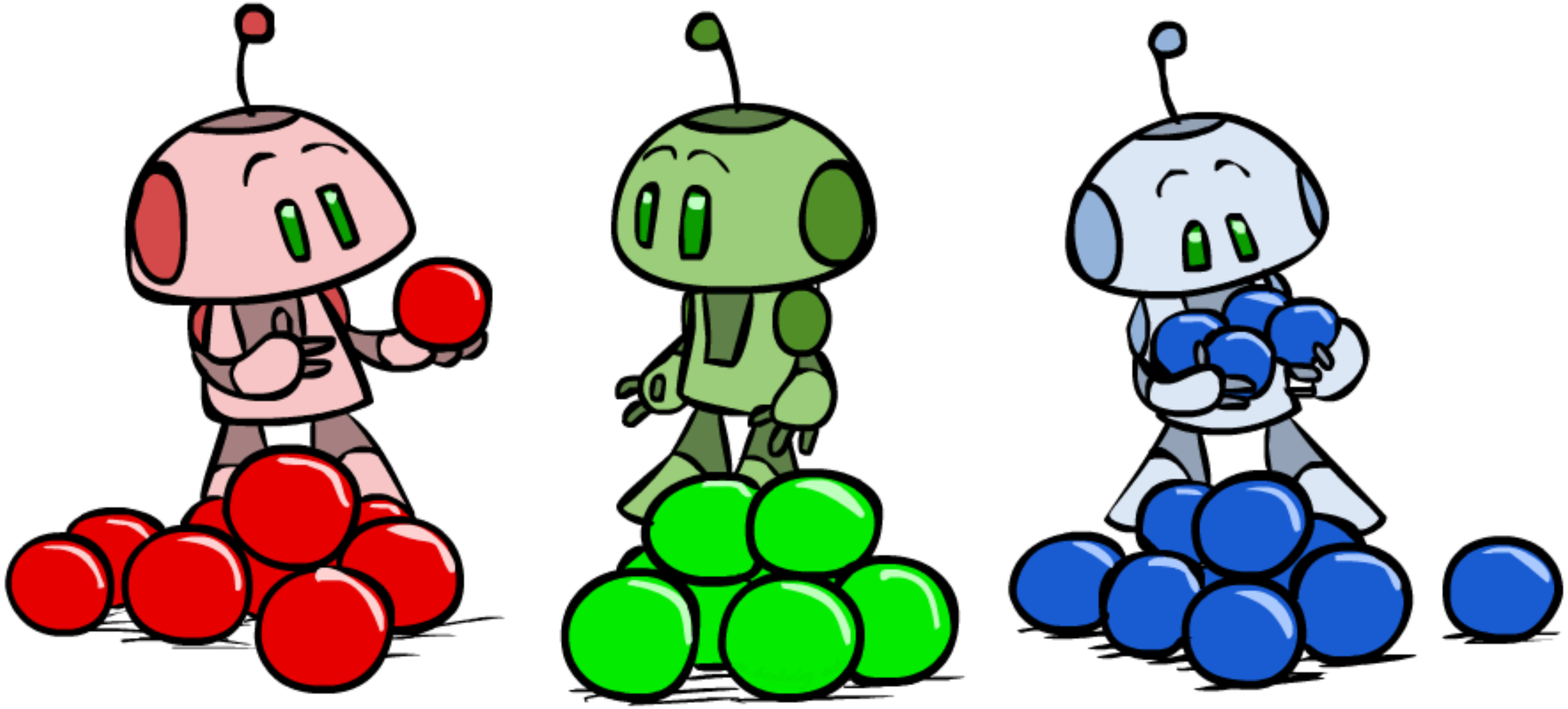
- Basic idea: group together similar instances
- Example: 2D point patterns



- What could "similar" mean?
  - One option: small (squared) Euclidean distance

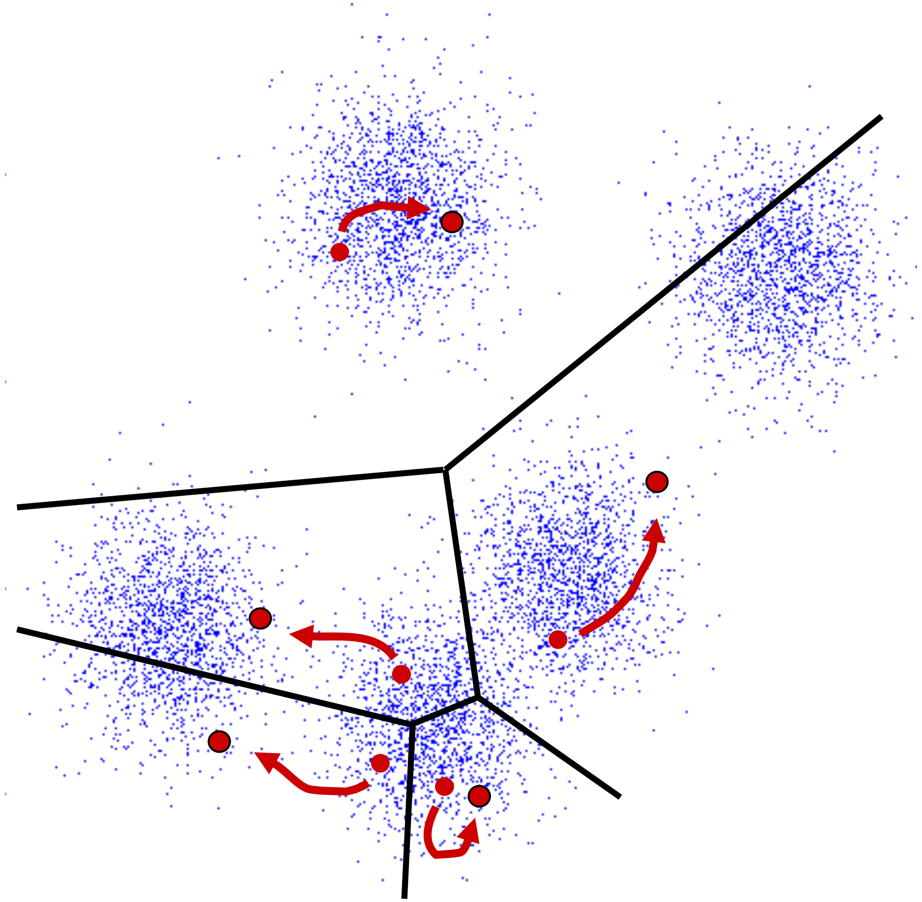
$$\text{dist}(x, y) = (x - y)^\top (x - y) = \sum_i (x_i - y_i)^2$$

K-Means

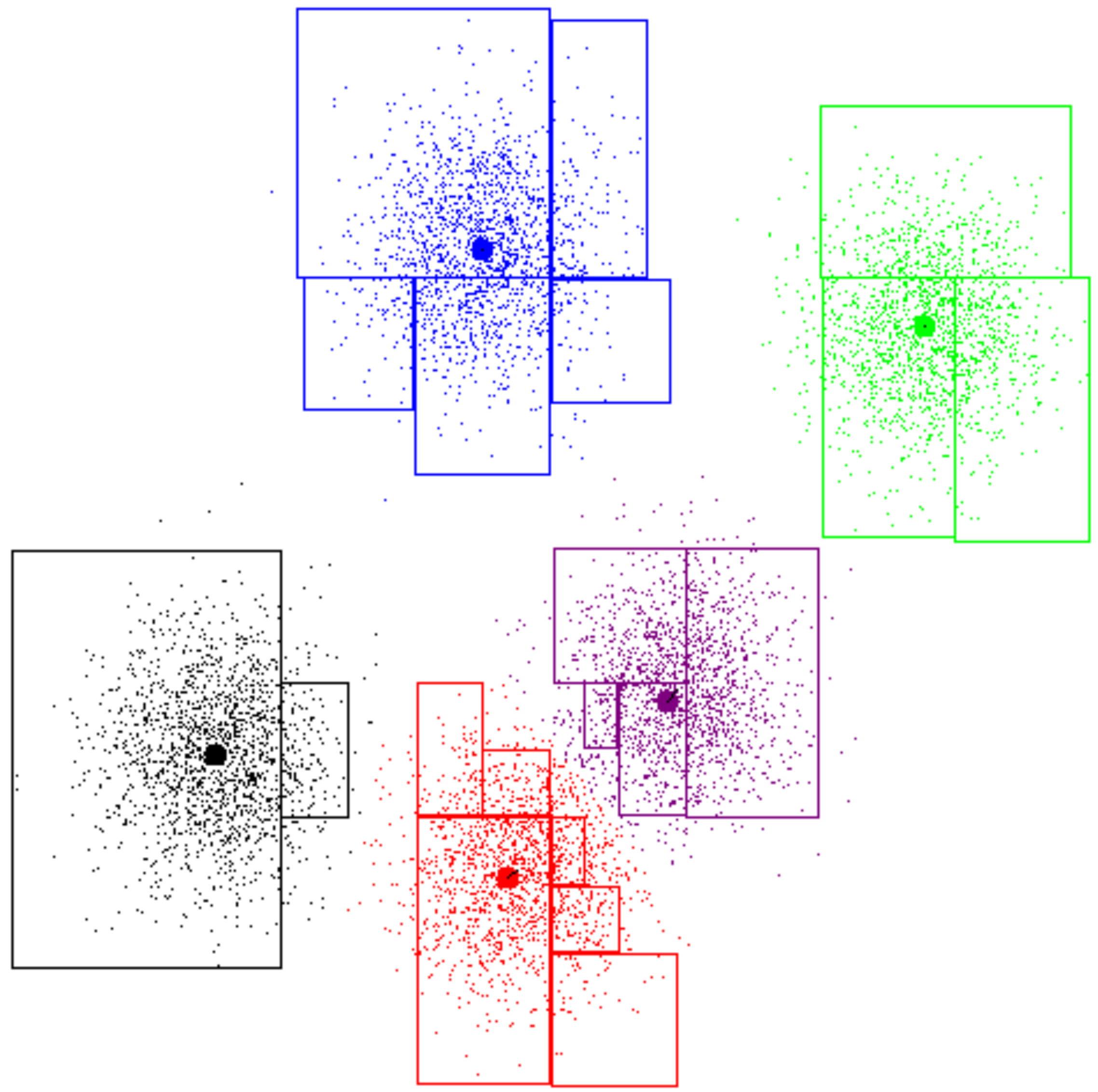


K-Means

- An iterative clustering algorithm
  - Pick K random points as cluster centers (means)
  - Alternate:
    - Assign data instances to closest mean
    - Assign each mean to the average of its assigned points
  - Stop when no points' assignments change



K-Means Example



K-Means as Optimization

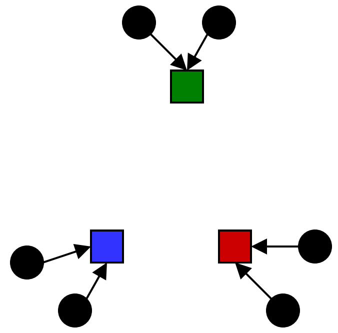
- Consider the total distance to the means:

$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

points

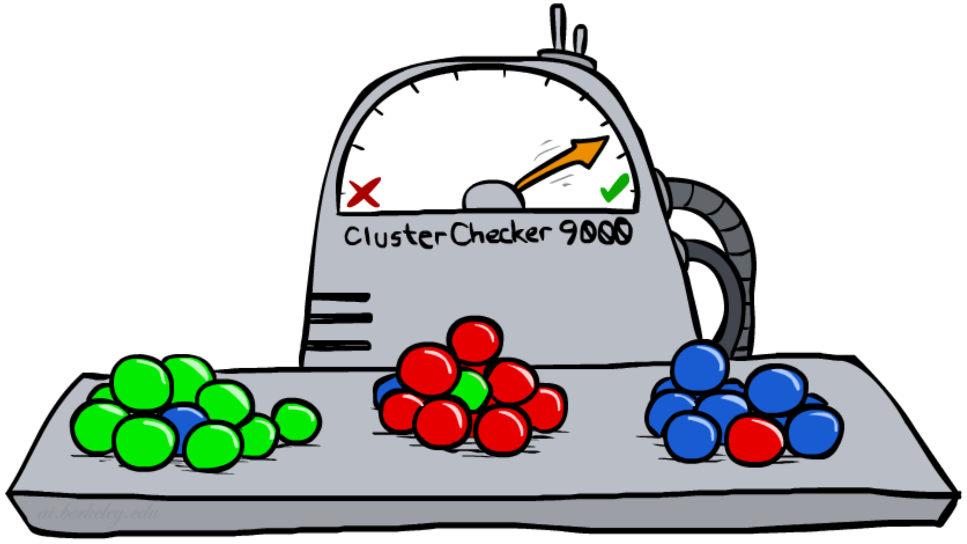
assignments

means



- Each iteration reduces phi

- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c



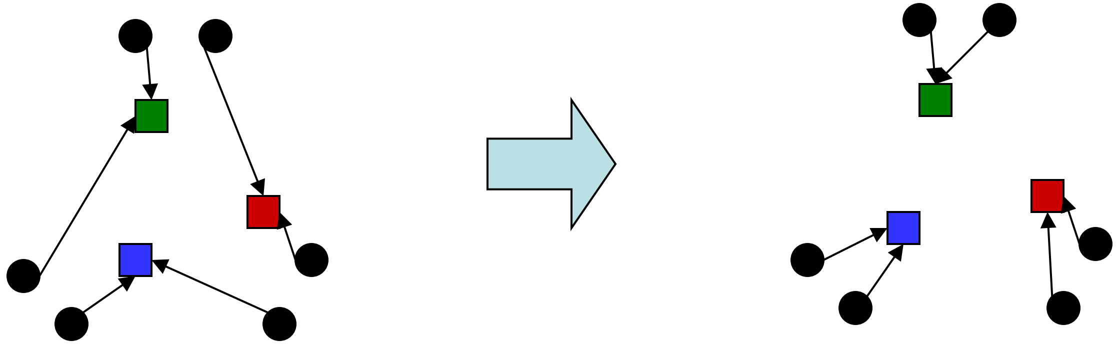
Phase I: Update Assignments

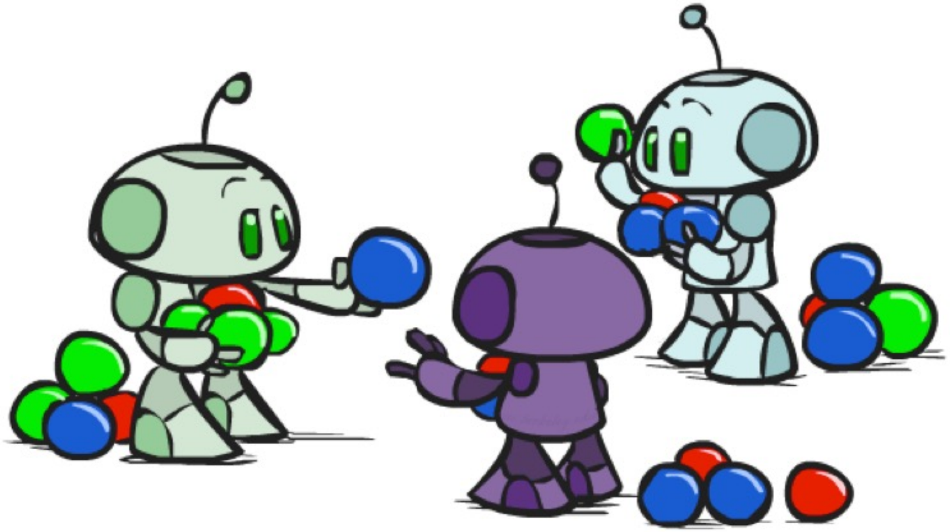
- For each point, re-assign to closest mean:

$$a_i = \underset{k}{\text{argmin}}\ \text{dist}(x_i, c_k)$$

- Can only decrease total distance phi!

$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$





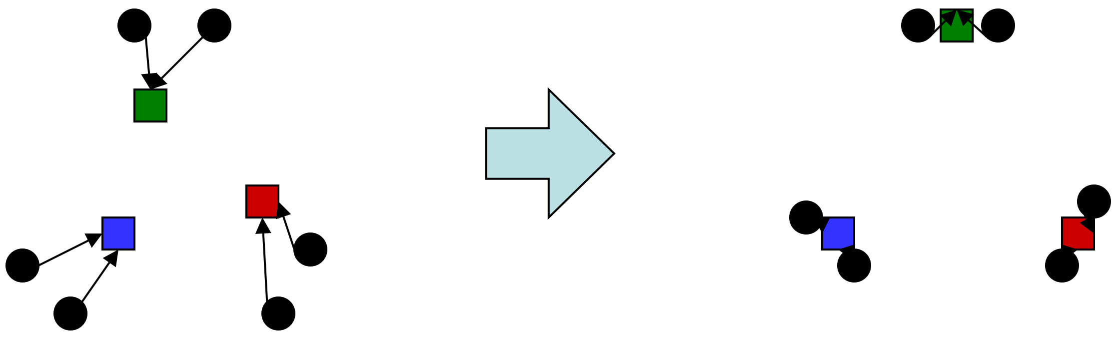
Phase II: Update Means

- Move each mean to the average of its assigned points:

$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$

- Also can only decrease total distance… (Why?)

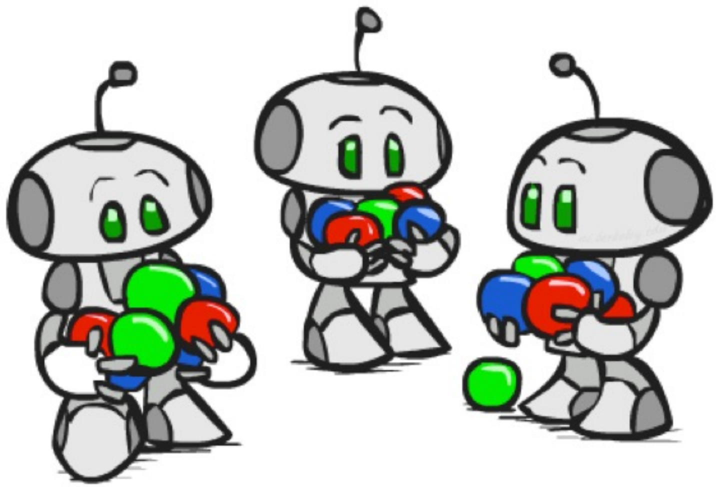
- Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean



Initialization

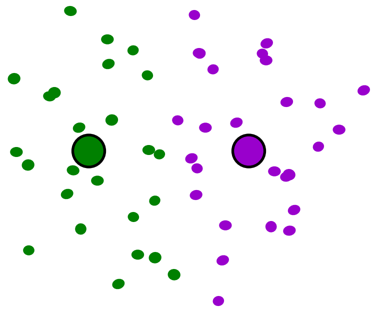
- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?

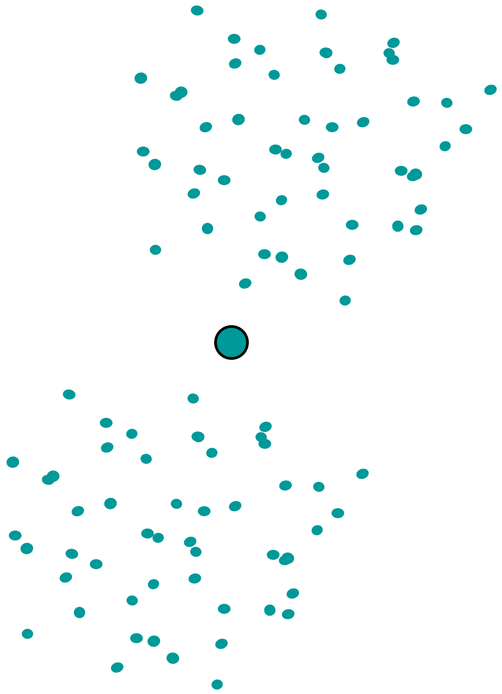
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics



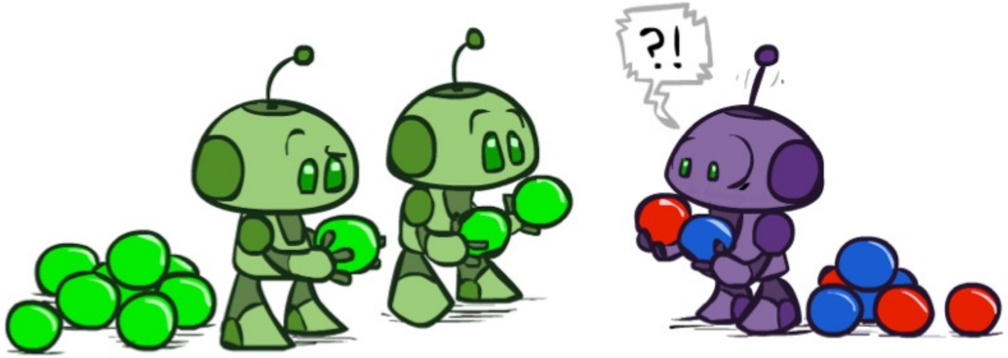
K-Means Getting Stuck

- A local optimum:



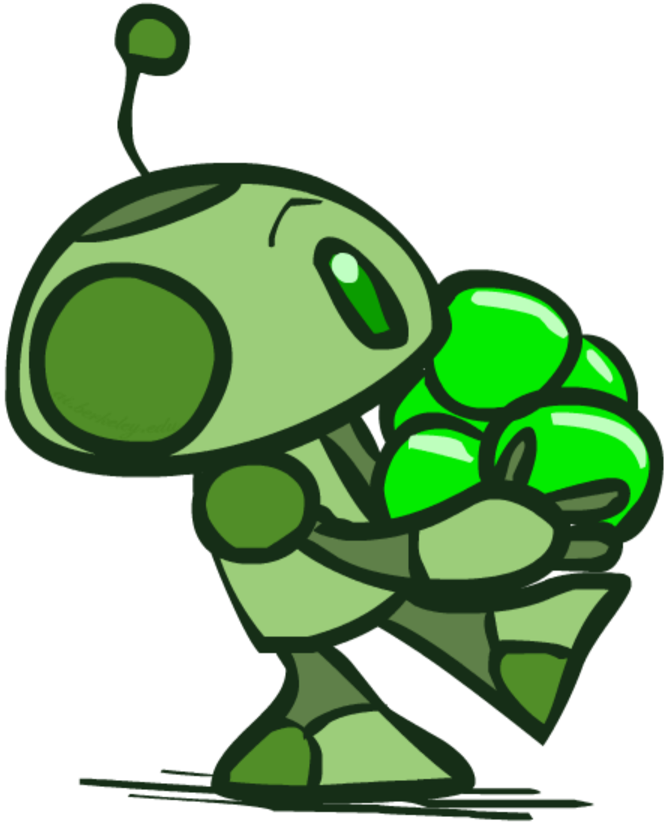


Why doesn't this work out like the earlier example, with the purple taking over half the blue?

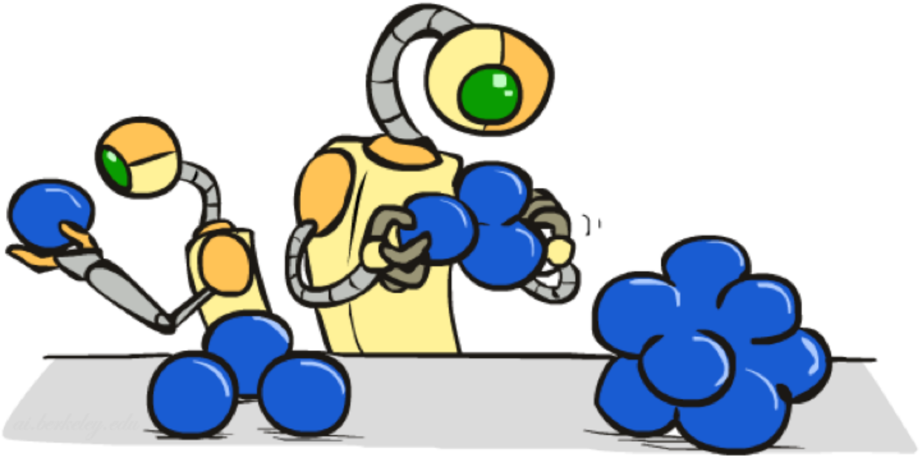


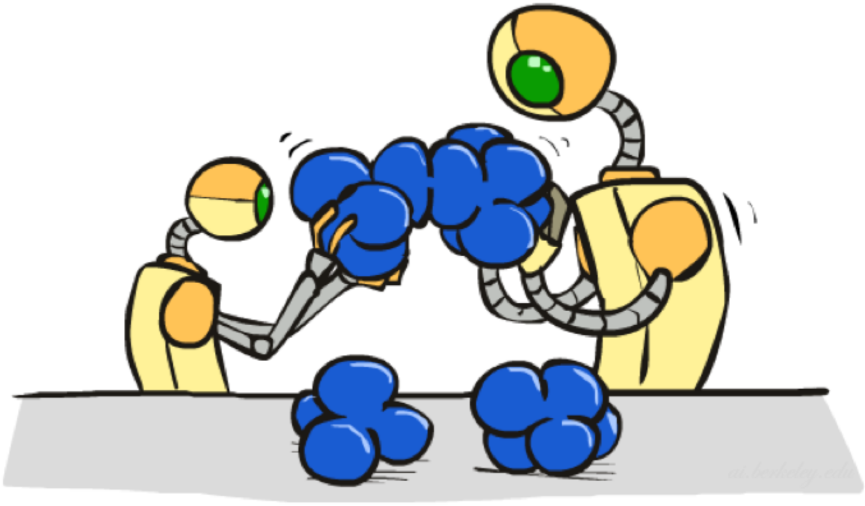
K-Means Questions

- Will K-means converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
  - If the patterns are very very clear?
- Will it find something interesting?
- Do people ever use it?
- How many clusters to pick?



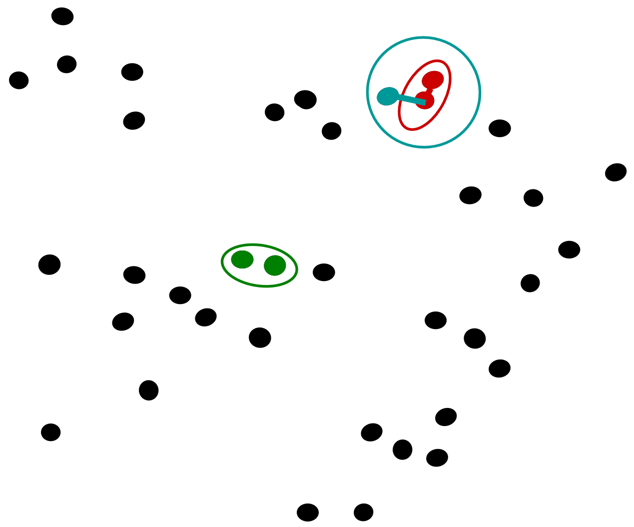
Agglomerative Clustering

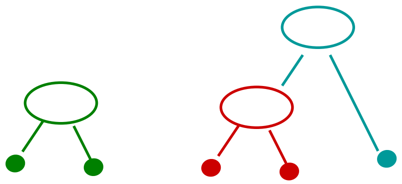




Agglomerative Clustering

- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left
- Produces not one clustering, but a family of clusterings represented by a dendrogram





Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?
- Many options
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs
  - Ward's method (min variance, like k-means)
- Different choices create different clustering behaviors