CS 188: Artificial Intelligence

ML Basics, Naïve Bayes

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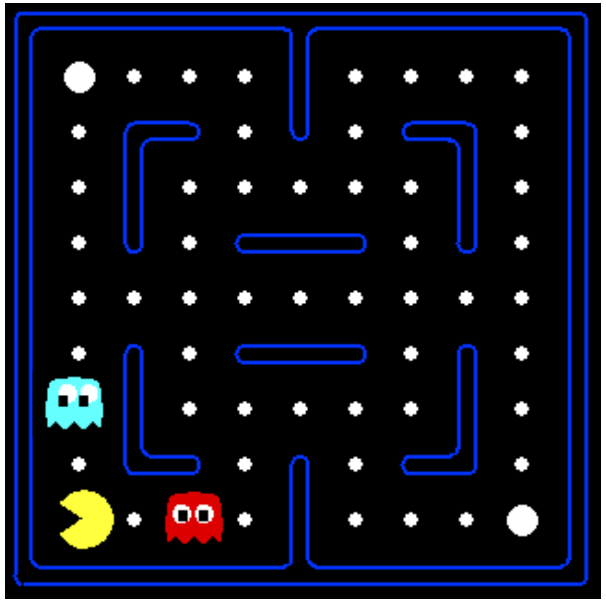
[These slides were created by Dan Klein, Pieter Abbeel, Anca Dragang, Sergey Levine, with some materials from A. Farhadi. All CS188 materials are at http://ai.berkeley.edu.]

Reinforcement Learning -- Overview

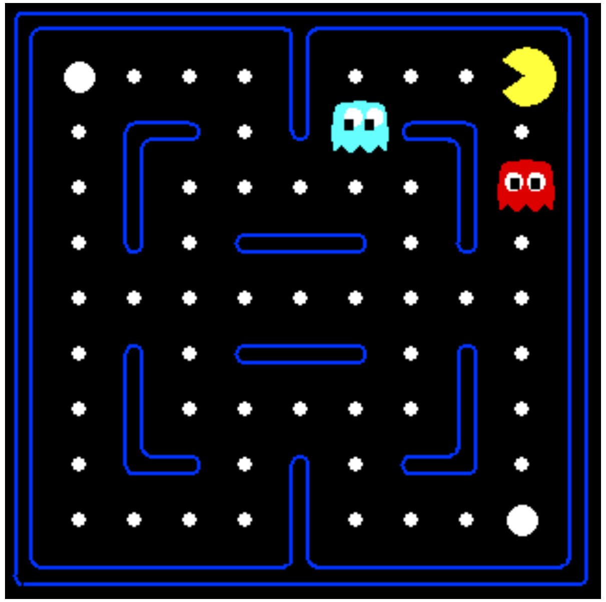
- Passive Reinforcement Learning (= how to learn from experiences)
  - Model-based Passive RL
    - Learn the MDP model from experiences, then solve the MDP
  - Model-free Passive RL
    - Forego learning the MDP model, directly learn V or Q:
      - Value learning – learns value of a fixed policy; 2 approaches: Direct Evaluation & TD Learning
      - Q learning – learns Q values of the optimal policy (uses a Q version of TD Learning)
- Active Reinforcement Learning (= agent also needs to decide how to collect experiences)
  - Key challenges:
    - How to efficiently explore?
    - How to trade off exploration <> exploitation
  - Applies to both model-based and model-free. In CS188 we'll cover only in context of Q-learning
- **Approximate Reinforcement Learning (= to handle large state spaces)**
  - **Approximate Q-Learning**
  - **Policy Search**

Example: Pacman

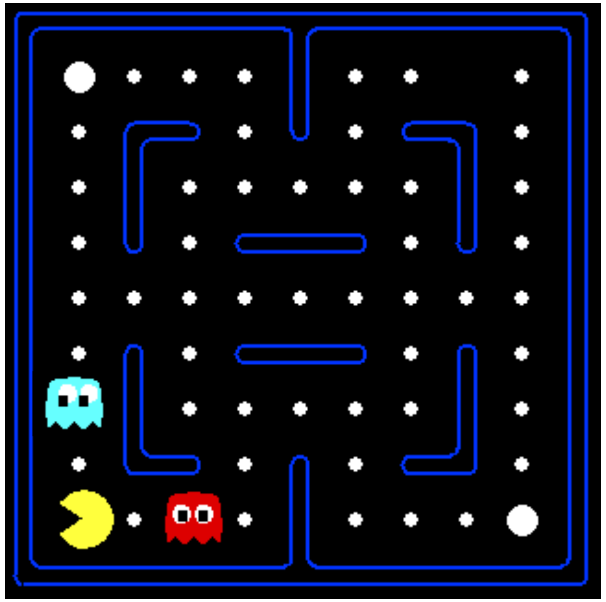
Let's say we discover through experience that this state is bad:



In naïve q-learning, we know nothing about this state:



Or even this one!



[Demo: Q-learning – pacman – tiny – watch all (L11D4)]
[Demo: Q-learning – pacman – tiny – silent train (L11D6)]
[Demo: Q-learning – pacman – tricky – watch all (L11D5)]

Approximate Q-Learning

$$Q(s,a) = w_1 f_1(s,a) + w_2 f_2(s,a) + \ldots + w_n f_n(s,a)$$

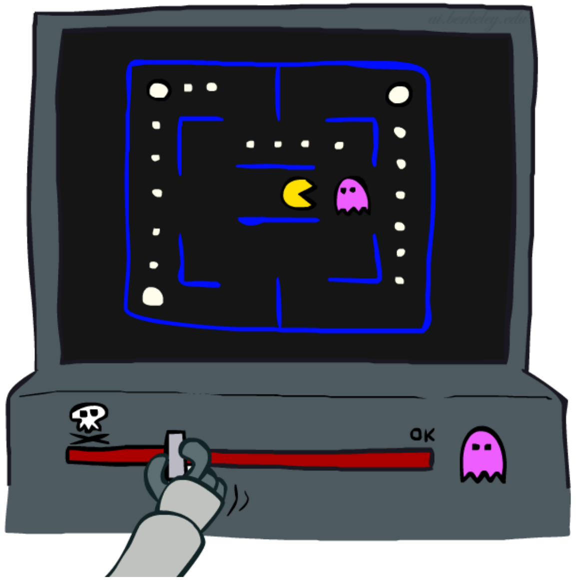
- Q-learning with linear Q-functions:

transition $= (s, a, r, s')$

difference $= \left[r + \gamma \max_{a'} Q(s', a') \right] - Q(s,a)$

$Q(s,a) \leftarrow Q(s,a) + \alpha$ [difference] Exact Q's

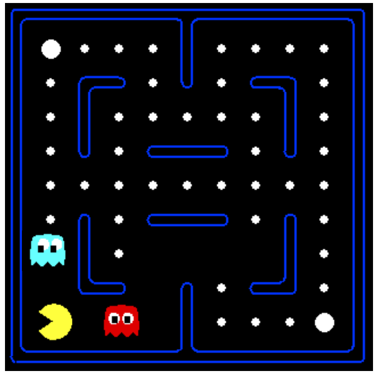
$w_i \leftarrow w_i + \alpha$ [difference] $f_i(s,a)$ Approximate Q's



Example: Q-Pacman

$$Q(s,a) = 4.0 f_{DOT}(s,a) - 1.0 f_{GST}(s,a)$$

s

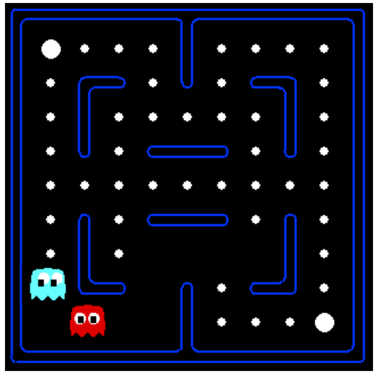


$f_{DOT}(s, \text{NORTH}) = 0.5$

$f_{GST}(s, \text{NORTH}) = 1.0$

$a = \text{NORTH}$
$r = -500$

s'



$Q(s, \text{NORTH}) = +1$

$r + \gamma \max_{a'} Q(s', a') = -500 + 0$

$Q(s', \cdot) = 0$

difference $= -501$

$w_{DOT} \leftarrow 4.0 + \alpha [-501] \, 0.5$

$w_{GST} \leftarrow -1.0 + \alpha [-501] \, 1.0$

$$Q(s,a) = 3.0 f_{DOT}(s,a) - 3.0 f_{GST}(s,a)$$

[Demo: approximate Q-learning pacman (L11D8)]

Video of Demo Approximate Q-Learning -- Pacman

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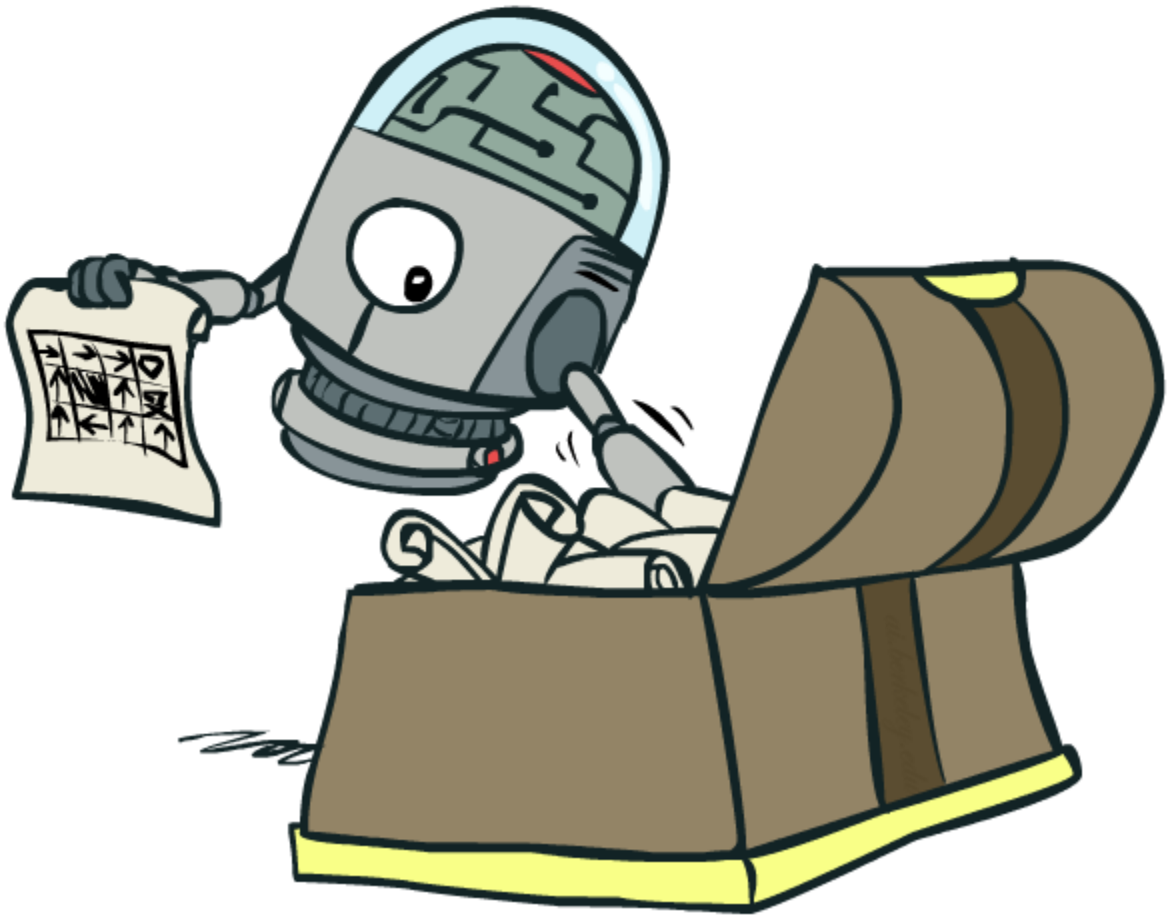
  - **Policy Search**

Policy Search



Policy Search

- Problem: often the feature-based policies that work well (win games, maximize utilities) aren’t the ones that approximate V / Q best
  - E.g. your value functions from project 2 were probably horrible estimates of future rewards, but they still produced good decisions
  - Q-learning’s priority: get Q-values close (modeling)
  - Action selection priority: get ordering of Q-values right (prediction)

- Solution: learn policies that maximize rewards, not the values that predict them

- Policy search: start with an ok solution (e.g. Q-learning) then fine-tune by hill climbing on feature weights

Policy Search

- Simplest policy search:
  - Start with an initial linear value function or Q-function
  - Nudge each feature weight up and down and see if your policy is better than before

- Problems:
  - How do we tell the policy got better?
  - Need to run many sample episodes!
  - If there are a lot of features, this can be impractical

- Better methods exploit lookahead structure, sample wisely, change multiple parameters…

To Summarize …

Known MDP: Offline Solution

Goal	Technique
Compute V*, Q*, π*	Value / policy iteration
Evaluate a fixed policy π	Policy evaluation

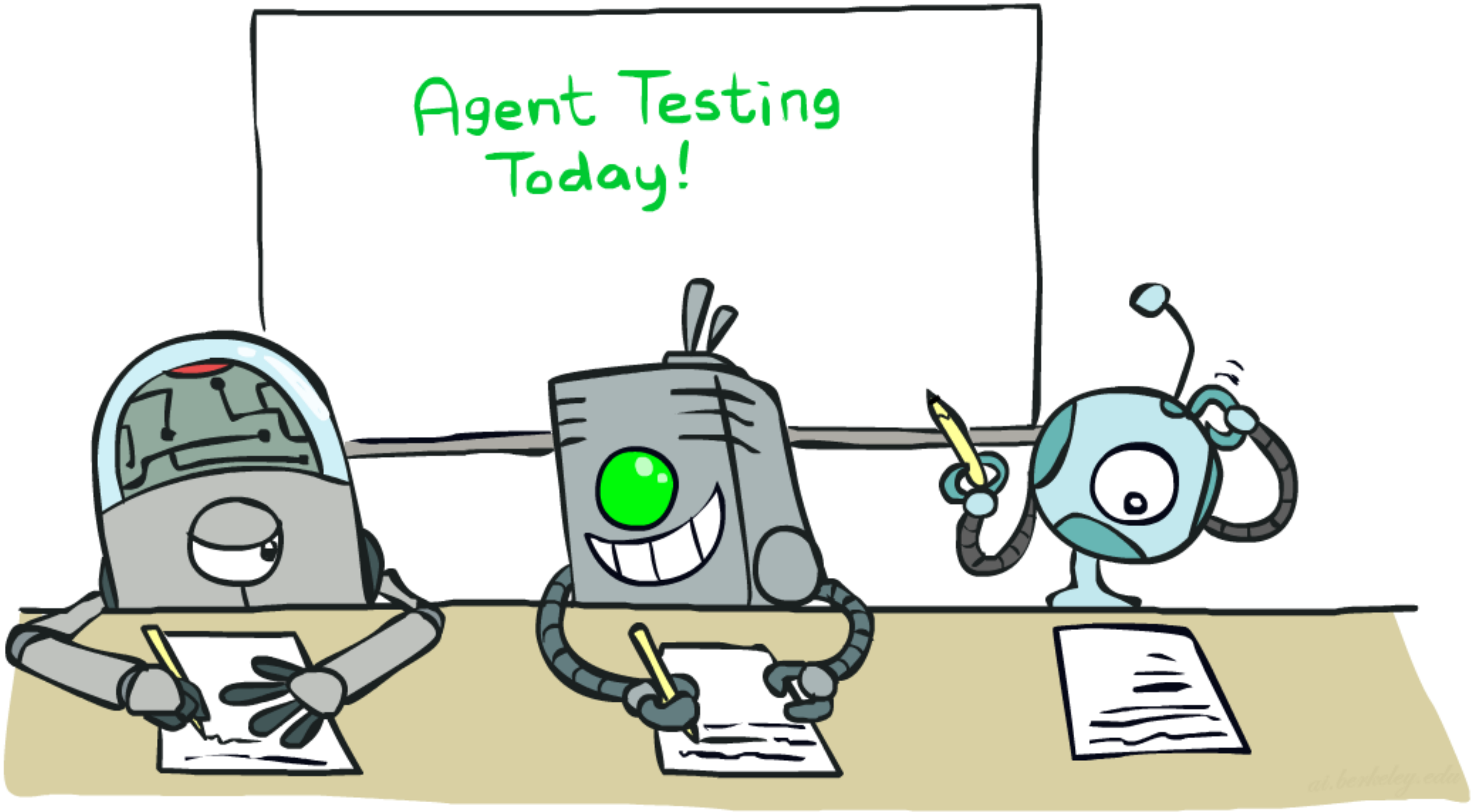
Unknown MDP: Model-Based

Goal	Technique
Compute V*, Q*, π*	VI/PI on approx. MDP
Evaluate a fixed policy π	PE on approx. MDP

Unknown MDP: Model-Free

Goal	Technique
Compute V*, Q*, π*	Q-learning
Evaluate a fixed policy π	Value Learning

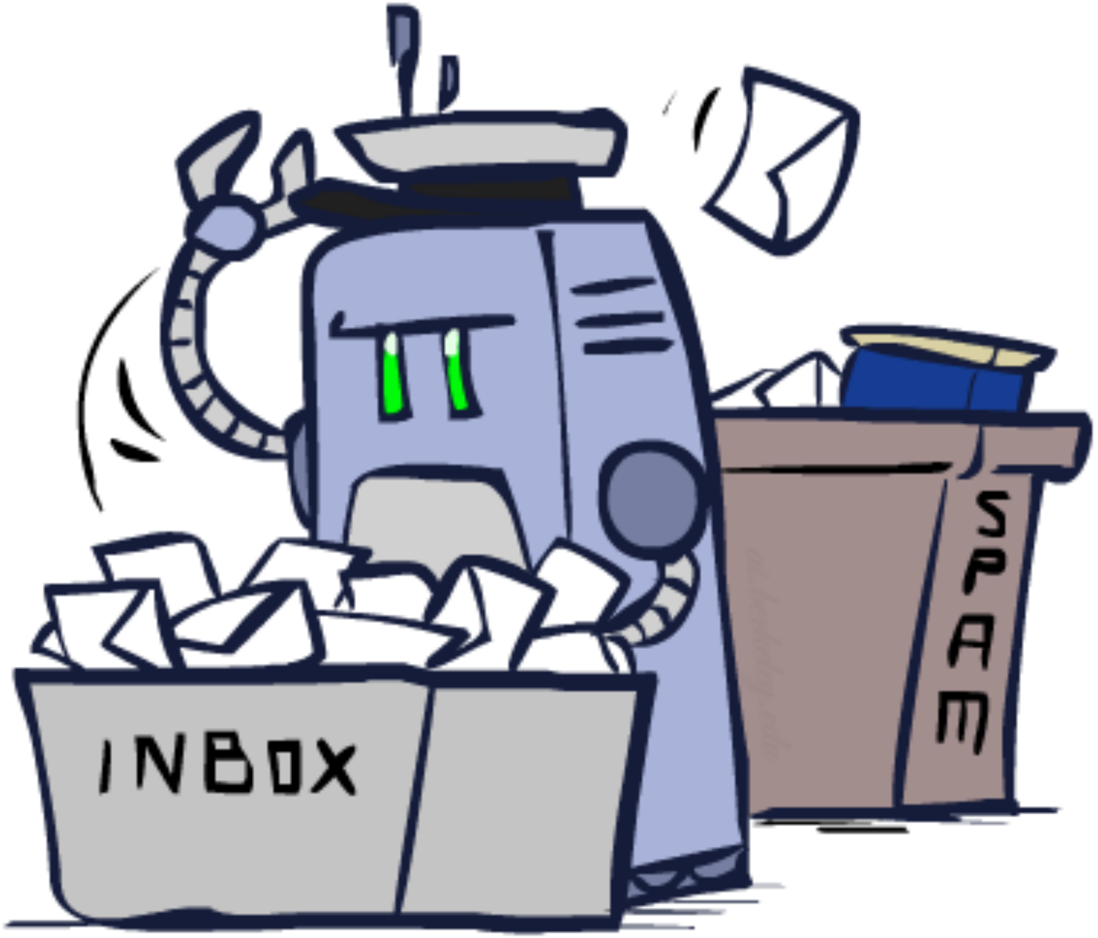
Machine Learning



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, 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. …

✗

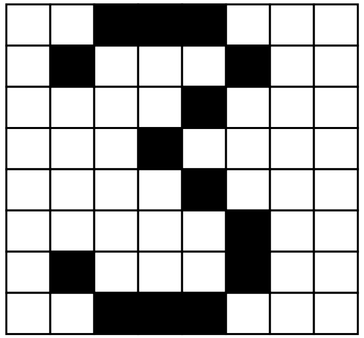
> TO BE REMOVED FROM FUTURE MAILINGS, SIMPLY REPLY TO THIS MESSAGE AND PUT "REMOVE" IN THE SUBJECT.
>
> 99 MILLION EMAIL ADDRESSES
> FOR ONLY $99

✓

> 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.

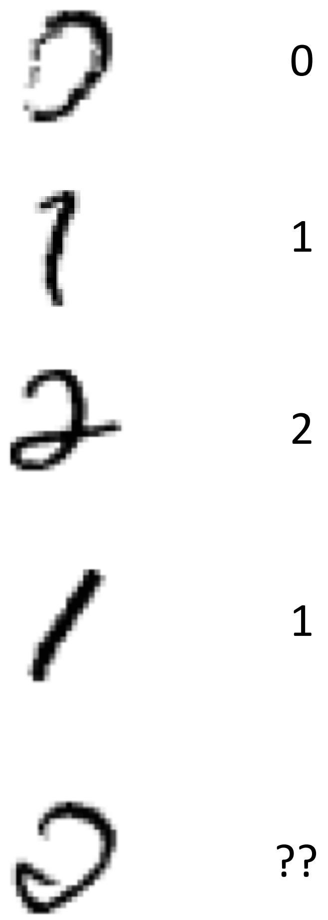
Example: Digit Recognition

- 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
  - …



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?

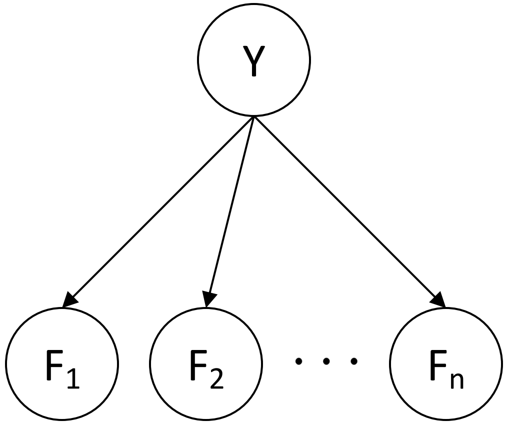
Naïve Bayes for Digits

- 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



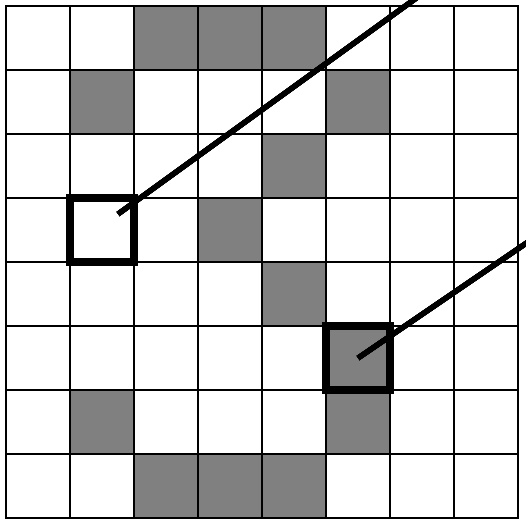
- Naïve Bayes model: $P(Y|F_{0,0} \ldots F_{15,15}) \propto P(Y) \prod_{i,j} P(F_{i,j}|Y)$

- What do we need to learn?

Naïve Bayes for Digits: 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



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

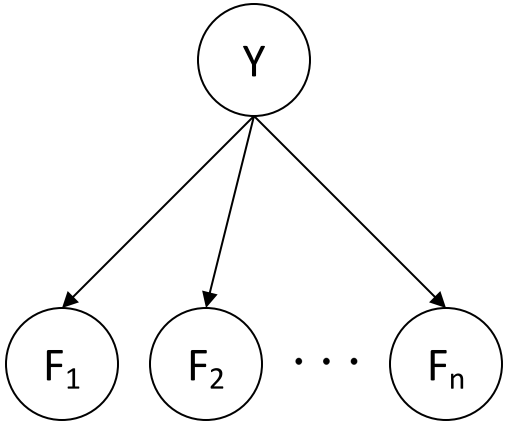
1	0.01
2	0.05
3	0.05
4	0.30
5	0.80
6	0.90
7	0.05
8	0.60
9	0.50
0	0.80

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

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

General Naïve Bayes

- A general Naive Bayes model:



|Y| parameters

$$P(Y, F_1 \dots F_n) = P(Y) \prod_i P(F_i|Y)$$

|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

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

$$+ \quad \longrightarrow \quad P(f_1 \ldots f_n)$$

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

$$\Downarrow$$

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

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

how many variables are there?
how many values?

- 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

Oh sorry I was still on mute

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
...	

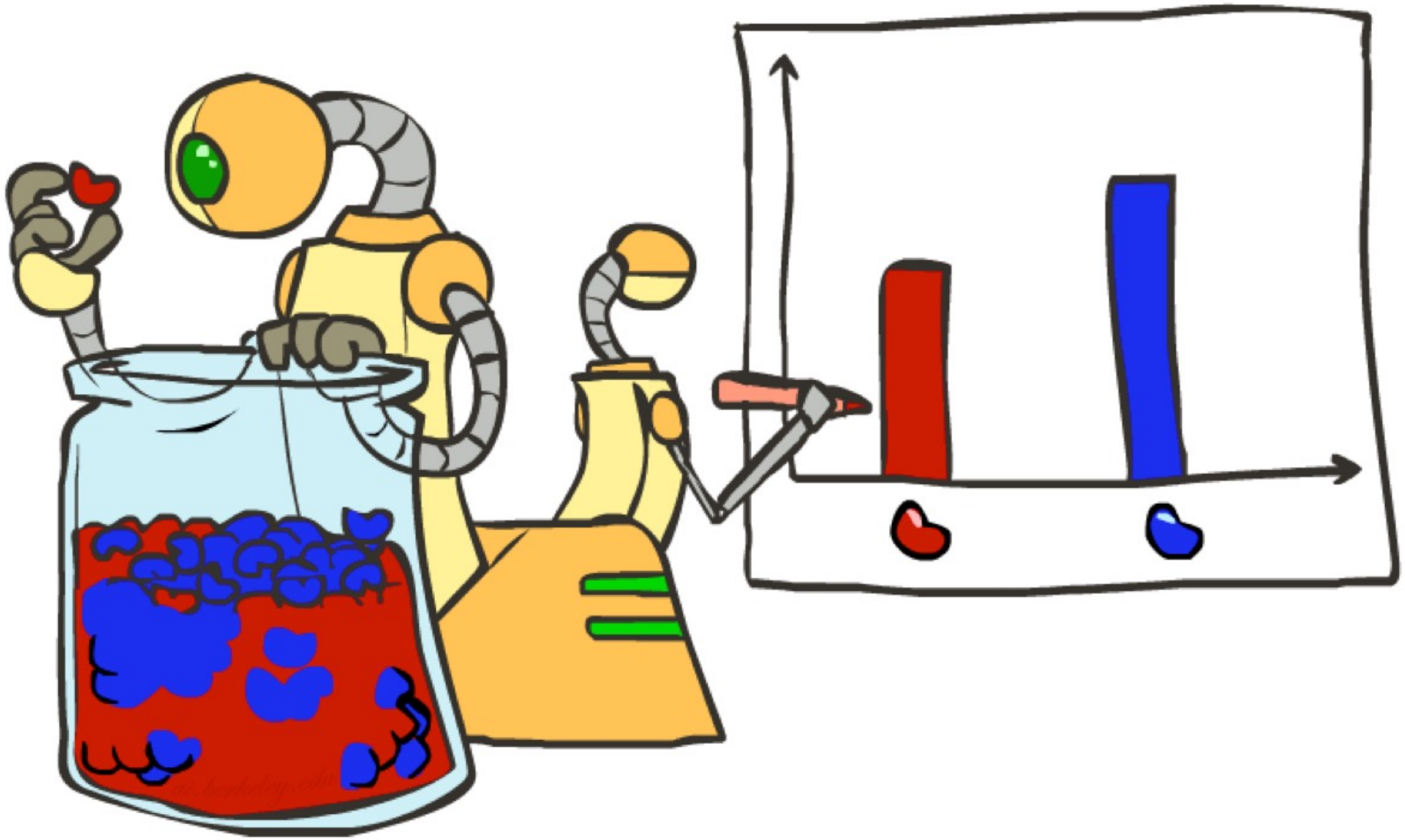
$P(W|\text{ham})$

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

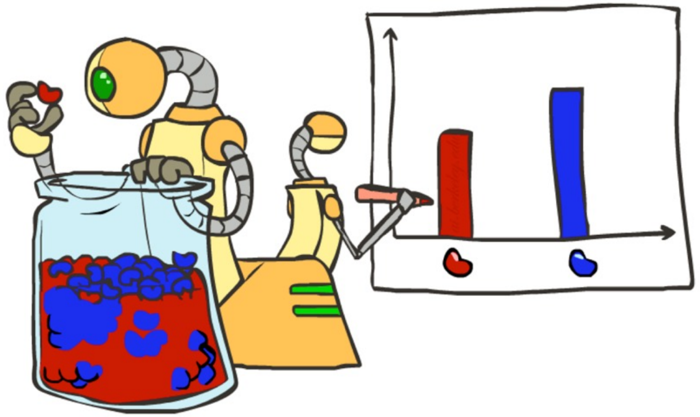
General Naïve Bayes

- What do we need in order to use Naïve Bayes?
  - Inference method
    - 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

Parameter Estimation



Parameter Estimation with Maximum Likelihood



- Estimating the distribution of a random variable
- *Option 1:* ask a human
- *Option 2:* 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 of the parameters that maximizes the *likelihood of the data*

$$L(x, \theta) = \prod_i P_\theta(x_i) = \theta \cdot \theta \cdot (1 - \theta)$$

$$P_\theta(x = \text{red}) = \theta$$

$$P_\theta(x = \text{blue}) = 1 - \theta$$

Parameter Estimation with Maximum Likelihood

- **Data:** Observed set D of α_H Heads and α_T Tails
- **Hypothesis space:** Binomial distributions
- **Learning:** finding θ is an optimization problem
  - What's the objective function?

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- **MLE:** Choose θ to maximize probability of *D*

$$\begin{aligned} \widehat{\theta} &= \arg\max_{\theta} \; P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \; \ln P(\mathcal{D} \mid \theta) \end{aligned}$$

Parameter Estimation with Maximum Likelihood

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} \ln P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\end{aligned}$$

- Set derivative to zero, and solve!

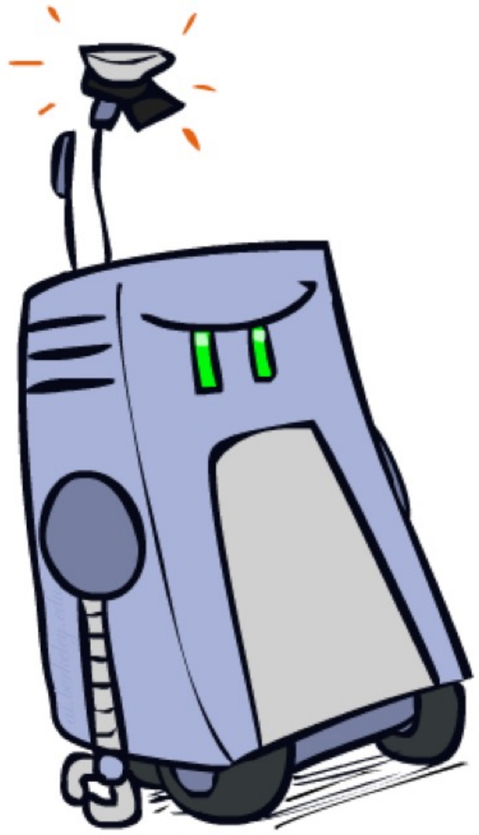
$$\begin{aligned}\frac{d}{d\theta} \ln P(\mathcal{D} \mid \theta) &= \frac{d}{d\theta}\left[\ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\right] \\ &= \frac{d}{d\theta}\left[\alpha_H \ln \theta + \alpha_T \ln(1-\theta)\right] \\ &= \alpha_H \frac{d}{d\theta} \ln \theta + \alpha_T \frac{d}{d\theta} \ln(1-\theta) \\ &= \frac{\alpha_H}{\theta} - \frac{\alpha_T}{1-\theta} = 0\end{aligned}$$

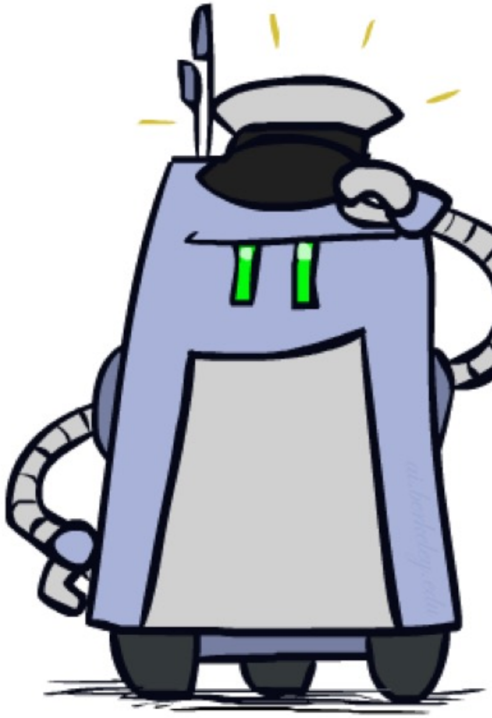
$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

Parameter Estimation with Maximum Likelihood

- How do we estimate the conditional probability tables?
  - Maximum Likelihood, which corresponds to counting
- Need to be careful though … let’s see what can go wrong..

Underfitting and Overfitting





Example: Overfitting

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

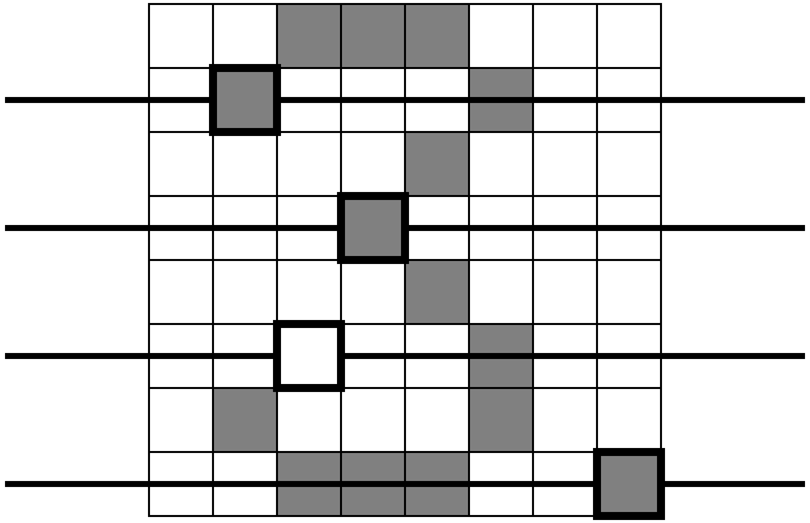
$P(C = 2) = 0.1$

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

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

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

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



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

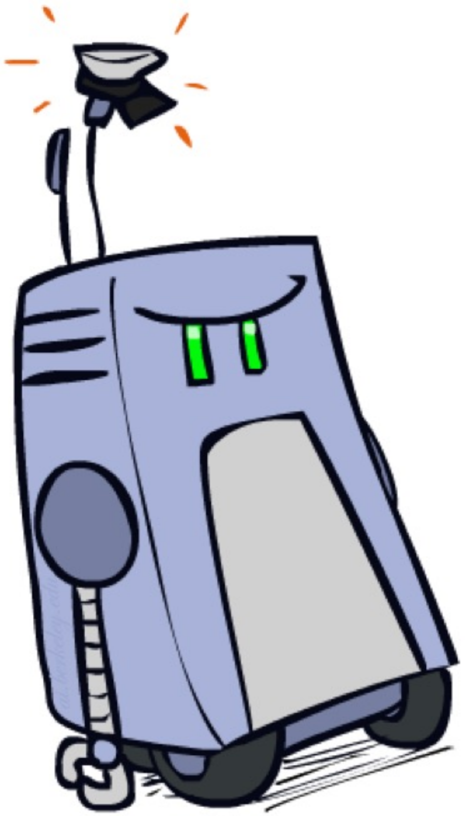
$P(C = 3) = 0.1$

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

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

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

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



2 wins!!

Example: Overfitting

- *relative* probabilities (odds ratios):

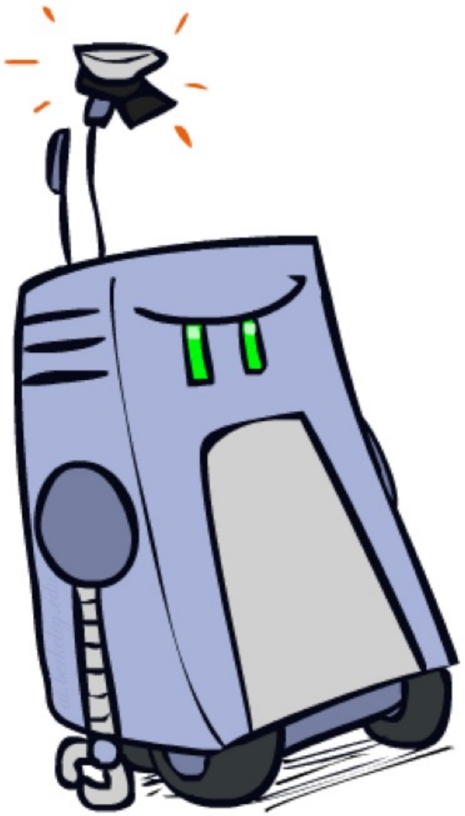
$$\frac{P(W|\text{ham})}{P(W|\text{spam})}$$

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

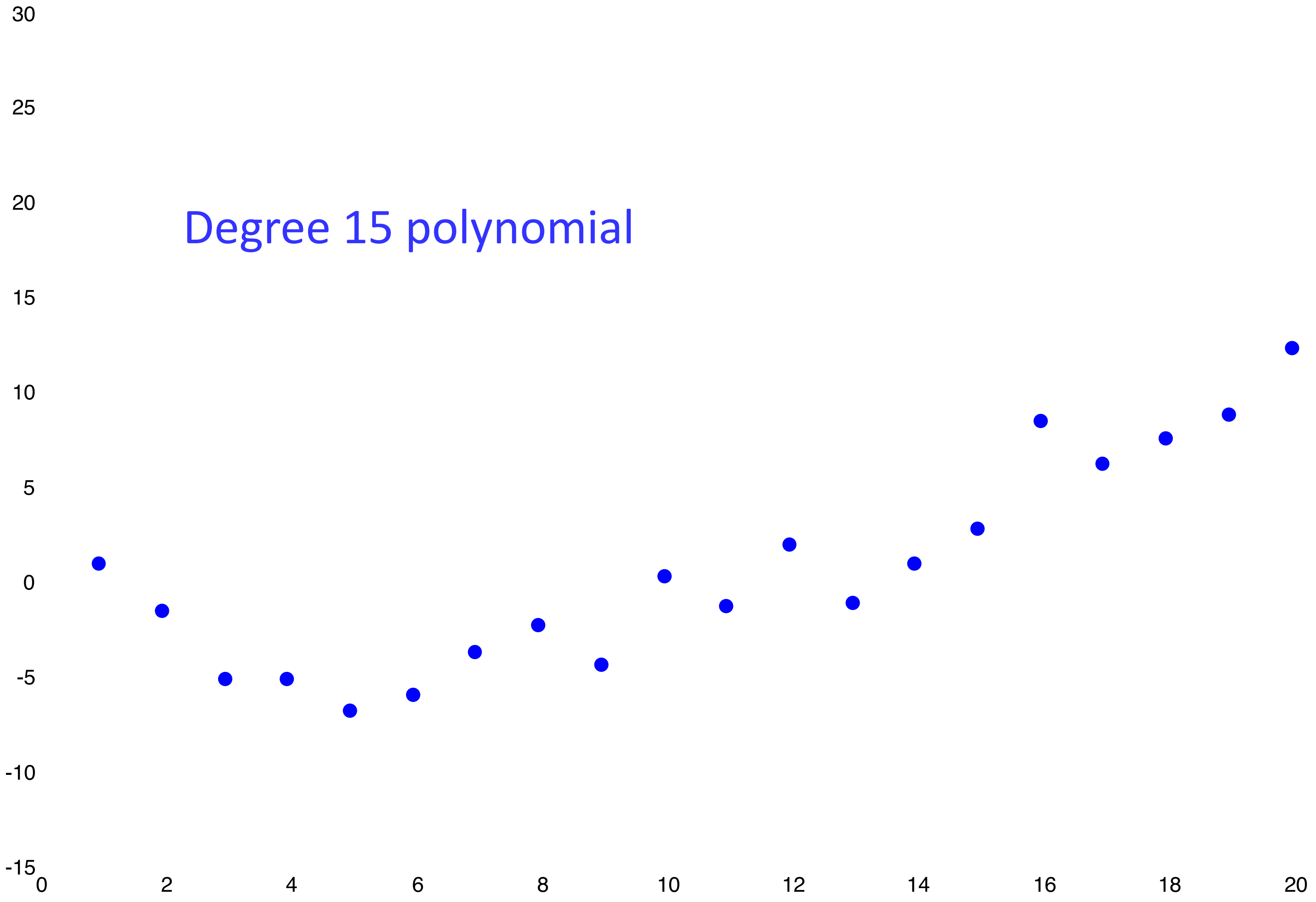
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

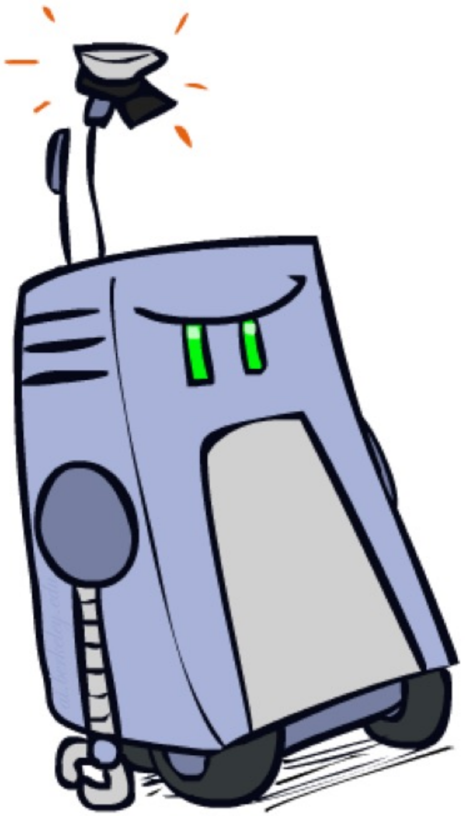
```
screens    : inf
minute     : inf
guaranteed : inf
$205.00    : inf
delivery   : inf
signature  : inf
...
```

What went wrong here?



Overfitting



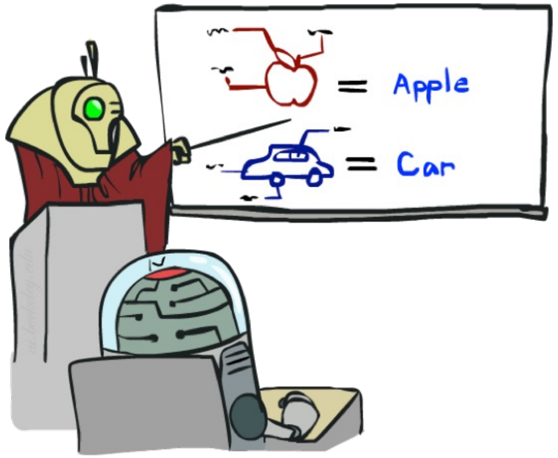


Training and Testing

Important Concepts

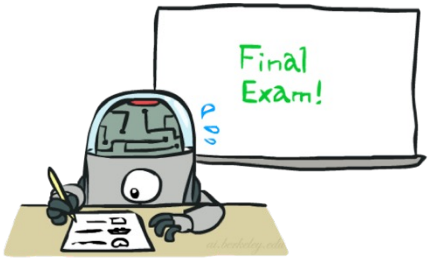
- Data: labeled instances, e.g. emails marked spam/ham
  - Training set
  - Held out set
  - Test set
- Features: attribute-value pairs which characterize each x
- Experimentation cycle
  - Learn parameters (e.g. model probabilities) on training set
  - (Tune hyperparameters on held-out set)
  - Compute accuracy on 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
  - <u>Overfitting</u>: fitting the training data very closely, but not generalizing well
  - <u>Underfitting</u>: fits the training set poorly

Training Data



Held-Out Data

Test Data



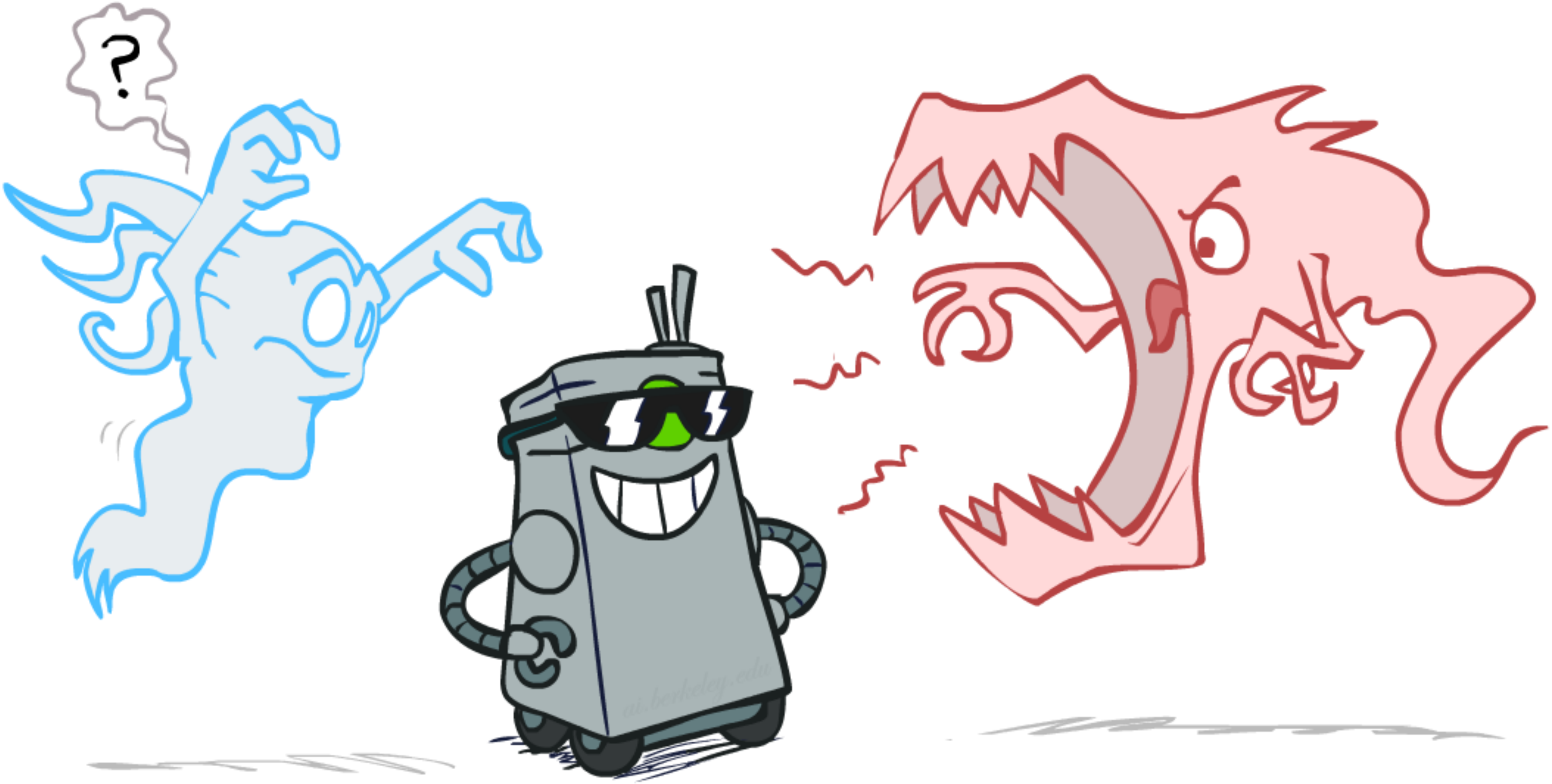
Generalization and Overfitting

- 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

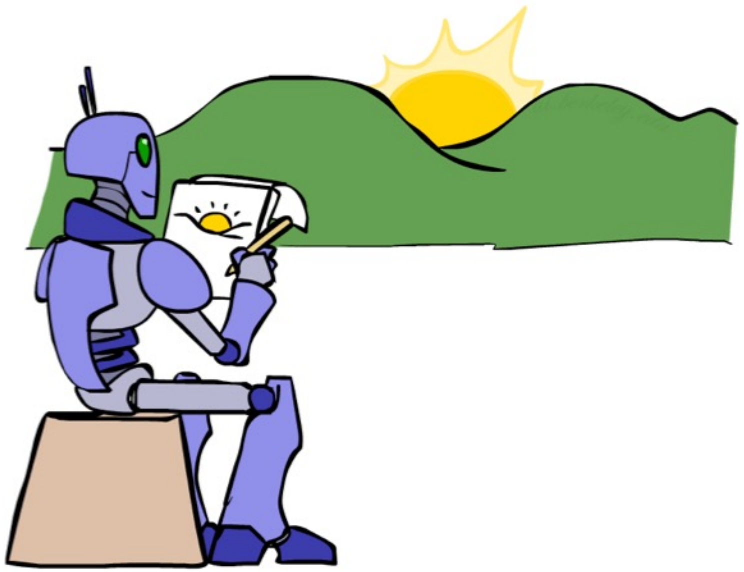
- As an extreme case, imagine using the entire email as the only feature
  - Would get the training data perfect (if deterministic labeling)
  - Wouldn't *generalize* at all
  - Just making the bag-of-words assumption gives us some generalization, but isn't enough

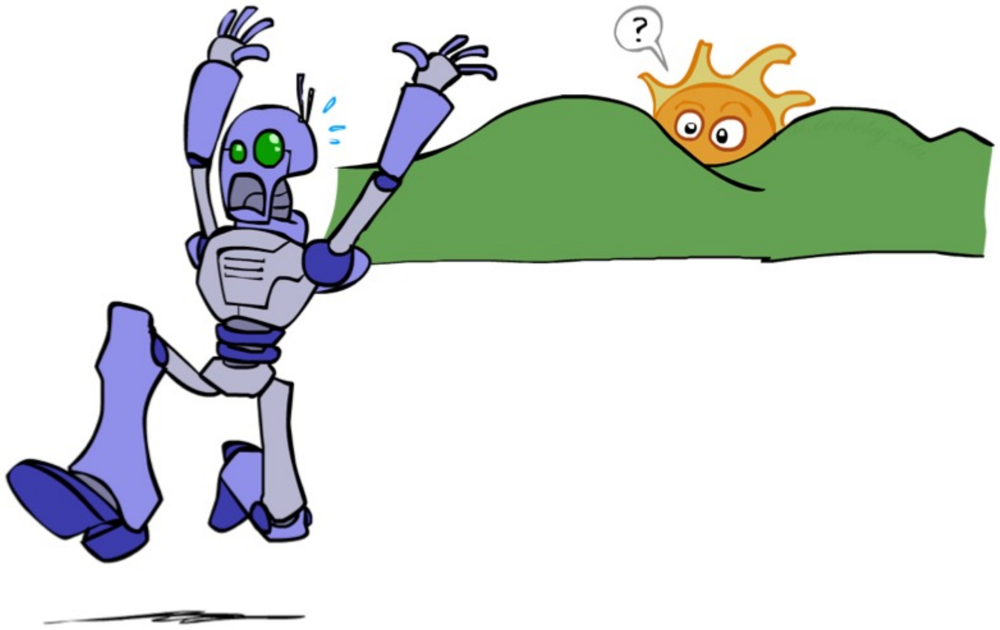
- To generalize better: we need to smooth or regularize the estimates

Smoothing



Unseen Events





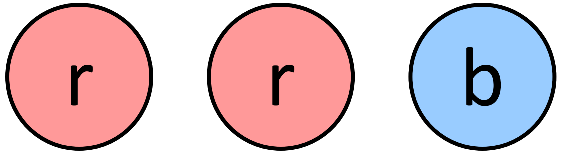
Laplace Smoothing

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

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

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

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



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

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

Laplace Smoothing

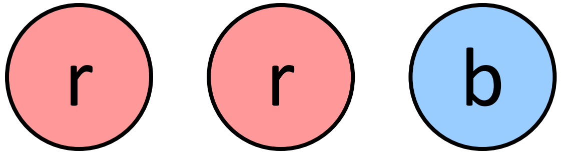
- Laplace's estimate (extended):
  - Pretend you saw every outcome k extra times

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

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

- Laplace for conditionals:
  - Smooth each condition independently:

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



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

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

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

Laplace Smoothing Can Be More Formally Derived

- Relative frequencies are the maximum likelihood estimates

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

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

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

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

⇒ “right” choice of P(theta)
-> Laplace estimates

Real NB: Smoothing

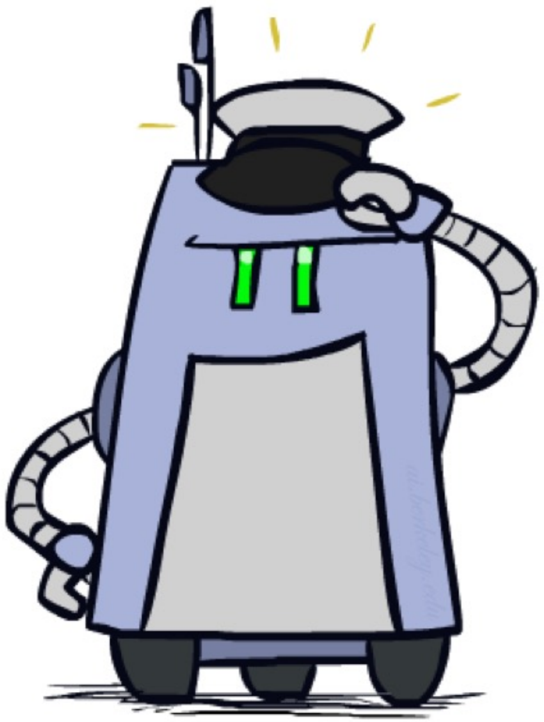
- For real classification problems, smoothing is critical
- New odds ratios:

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

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

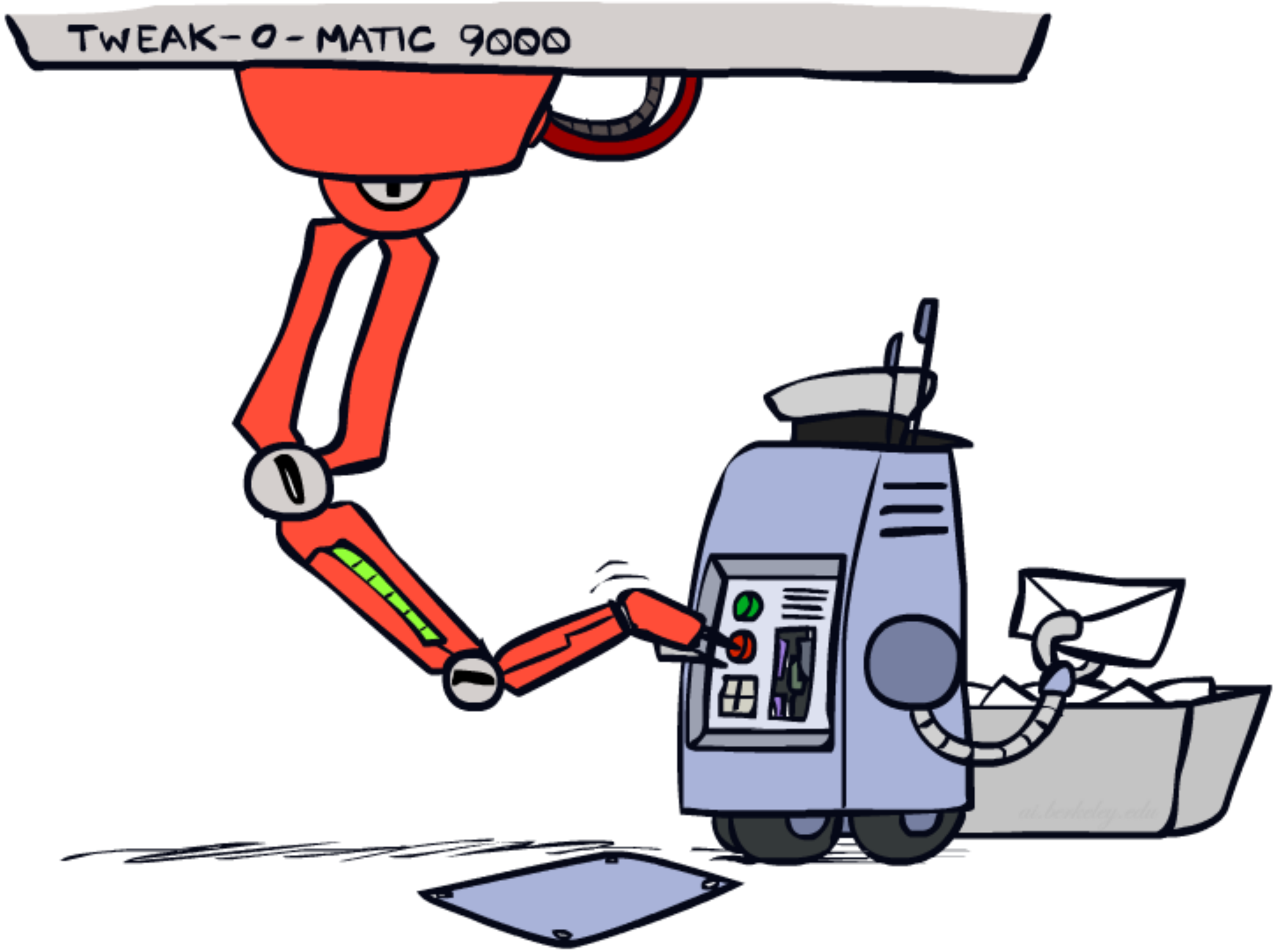
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

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



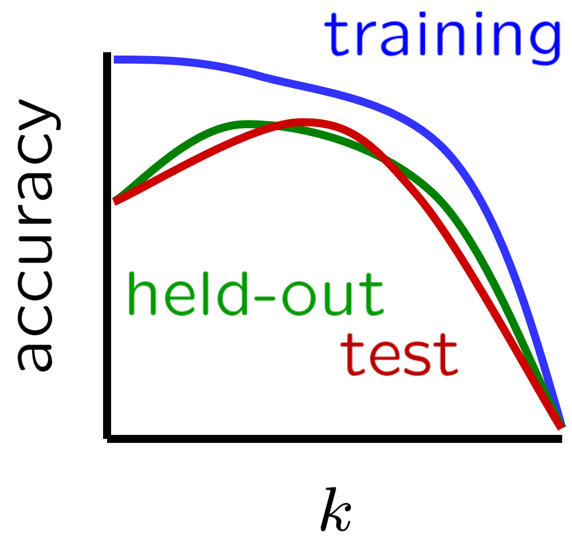
Do these make more sense?

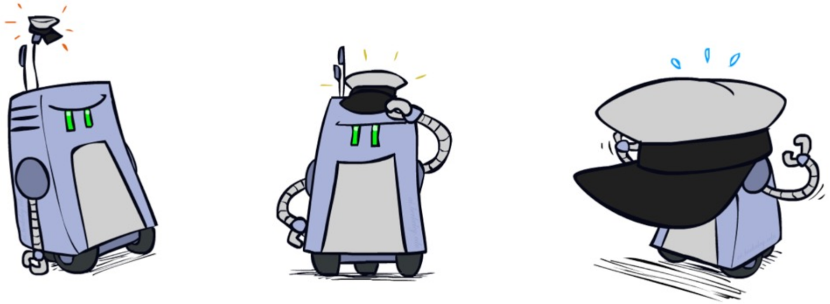
Tuning



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





Practical Tip: 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

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