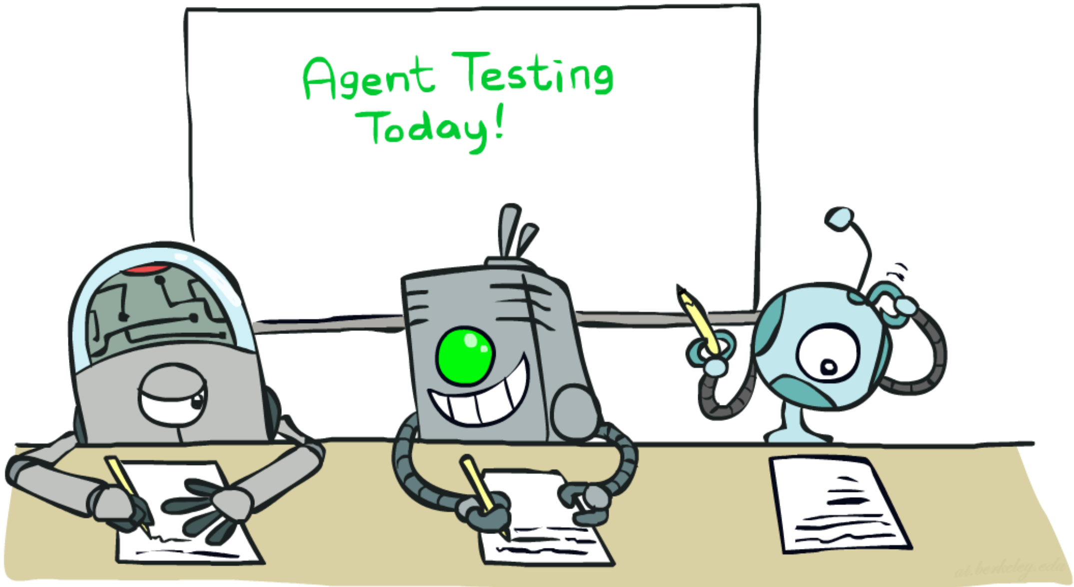
Artificial Intelligence - INFOF311

ML and naïve bayes

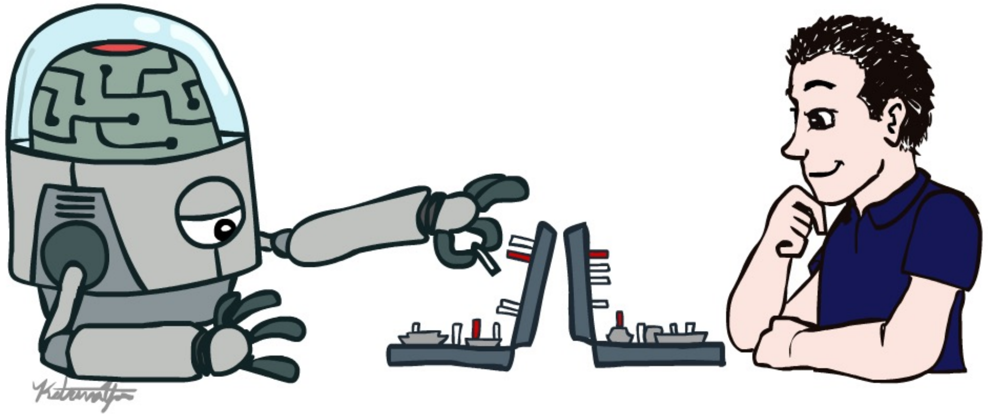


Instructor : Tom Lenaerts

Acknowledgement

We thank Stuart Russell for his generosity in allowing us to use the slide set of the UC Berkeley Course CS188, Introduction to Artificial Intelligence. These slides were created by Dan Klein, Pieter Abbeel and Anca Dragan for CS188 Intro to AI at UC Berkeley. All CS188 materials are available at http://ai.berkeley.edu.

Center for Human-Compatible Artificial Intelligence



The slides for INFOF311 are slightly modified versions of the slides of the spring and summer CS188 sessions in 2021 and 2022

Aims of the course

4 main themes :

Part 1 : Search and planning (uninformed and informed search, local search, game and adversarial search, …)

Part 2: Probabilistic reasoning (Bayesian network, hidden Markov models, filtering, decision networks…)

Part 3: Decision making with uncertainty (MDP, reinforcement learning, …)

Part 4: Machine learning (naïve bayes, perceptrons, regression, neural networks, …)

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

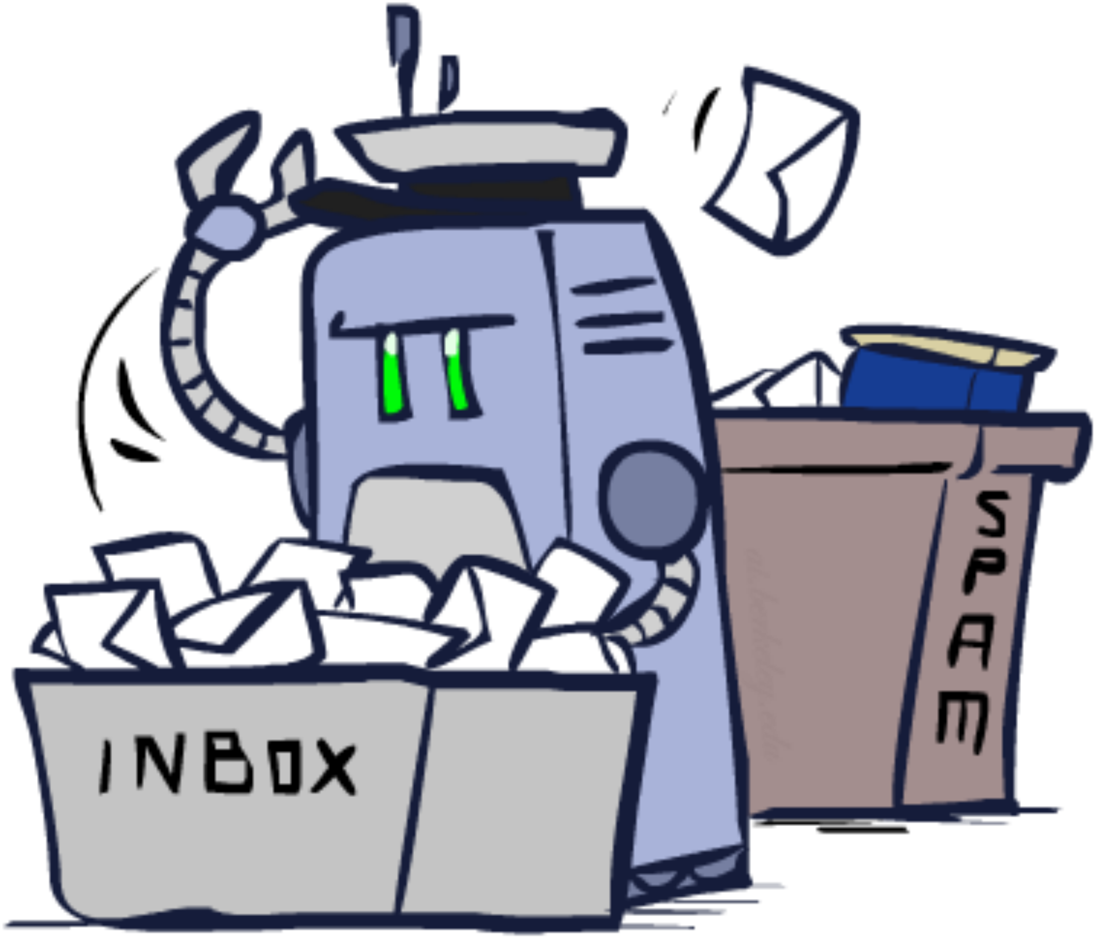
The roadmap

- Define the problem
  - Type of problems, domains (i.e. spam filtering, digit recognition)
- Look at several learning approaches/models
  - Naïve bayes, perceptrons, logistic regression and neural networks
- How to find model parameters; Maximum likelihood
  - Special cases; solved analytically
  - In general; numerical optimization
- Themes throughout
  - Workflow and working with data
  - Overfitting and smoothing
  - Evaluation: tracking and forecasting progress
  - applications

Multiple learning problems

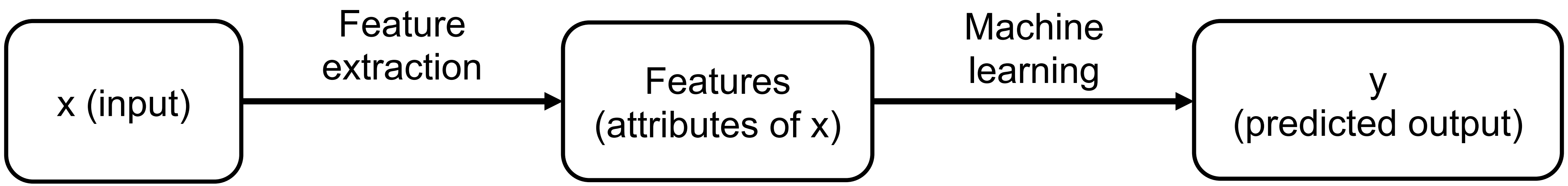
- Supervised learning: correct answers for each training instance
  - Classification: learning predictor with discrete outputs
  - Regression: learn predictor with real-valued outputs
- Reinforcement learning: reward sequence, no correct answers
- Unsupervised learning: “just make sense of the data”

Classification



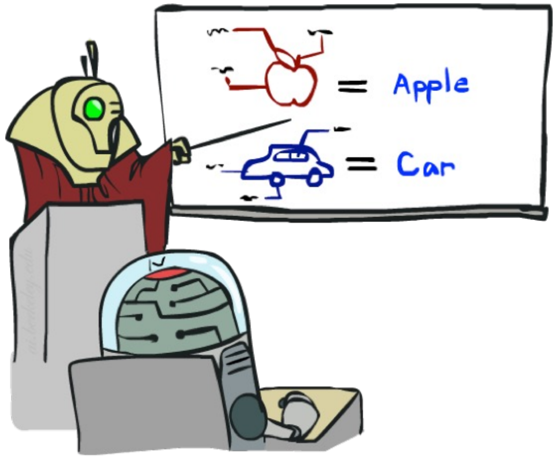
Classification and Machine Learning

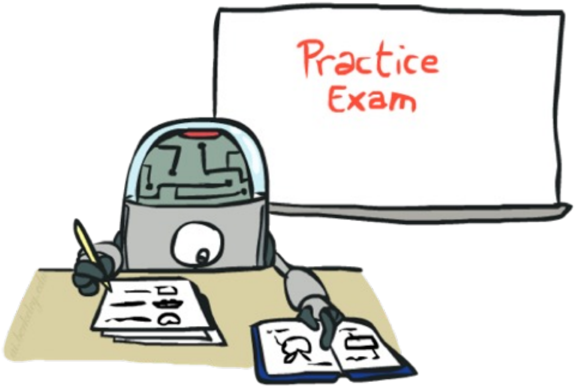
- Dataset: each data point, x, is associated with some label (aka class), y
- Goal of classification: given inputs x, write an algorithm to predict labels y
- Workflow of classification process:
  - Input is provided to you
  - Extract **features** from the input: attributes of the input that characterize each x and hopefully help with classification
  - Run some machine learning algorithm on the features: today, Naïve Bayes
  - Output a predicted label y

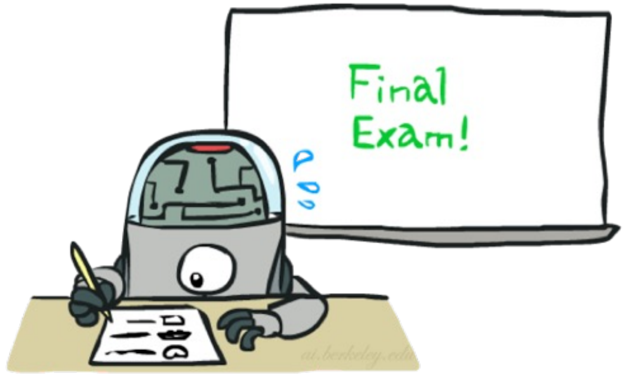


Training and Machine Learning

- Big idea: ML algorithms learn patterns between features and labels from *data*
  - You don't have to reason about the data yourself
  - You're given **training data**: lots of example datapoints and their actual labels







Training: Learn patterns from labeled data, and periodically test how well you're doing

Eventually, use your algorithm to predict labels for unlabeled data

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.

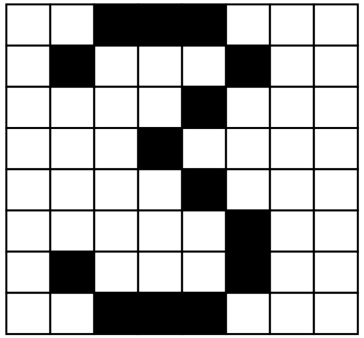
99 MILLION EMAIL ADDRESSES
FOR ONLY $99

✓

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
  - …

0

1

2

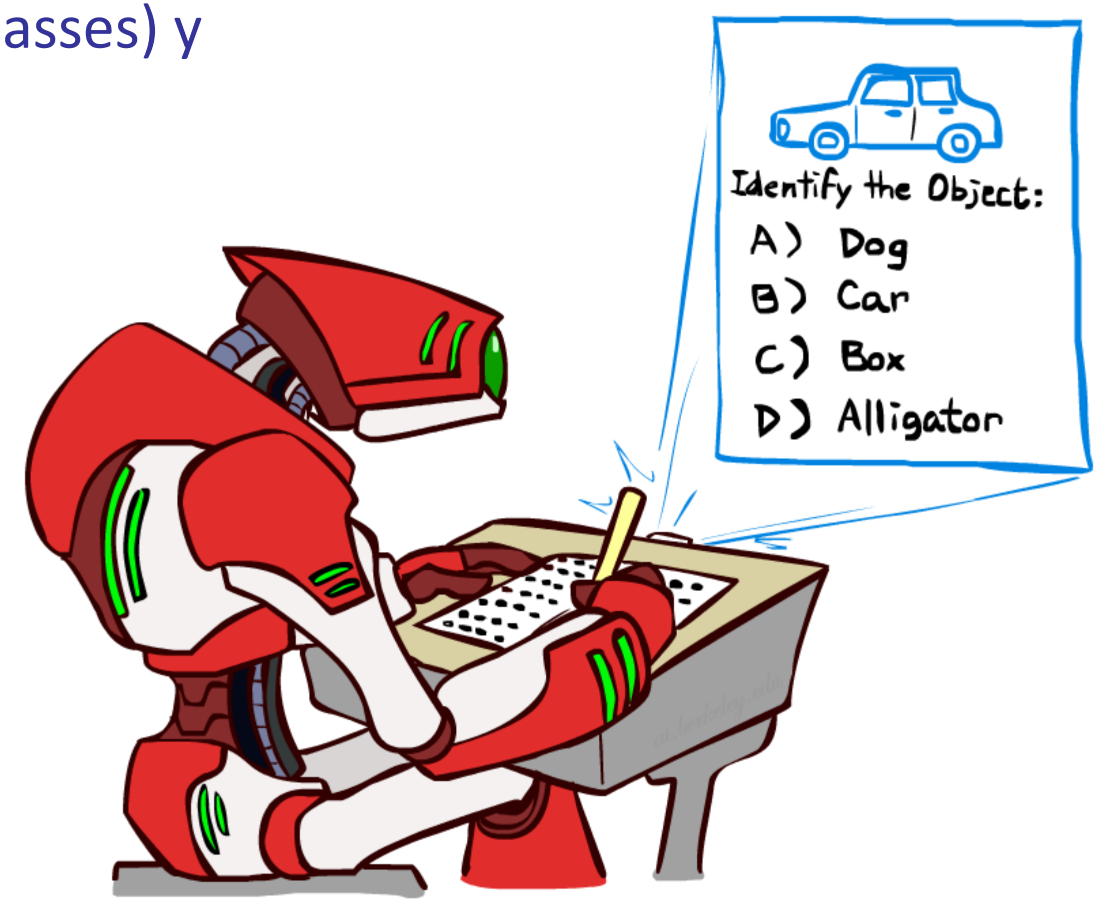
1

??

Other Classification Tasks

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

- 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

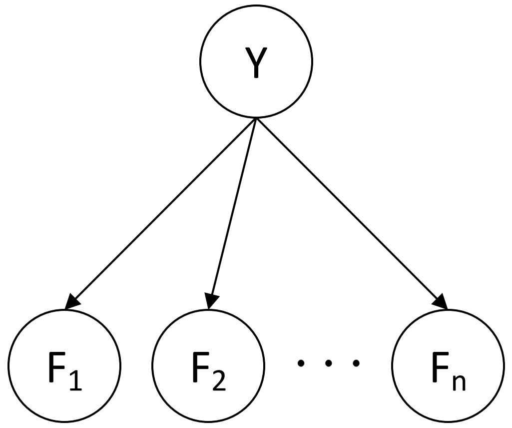
Model-Based Classification

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

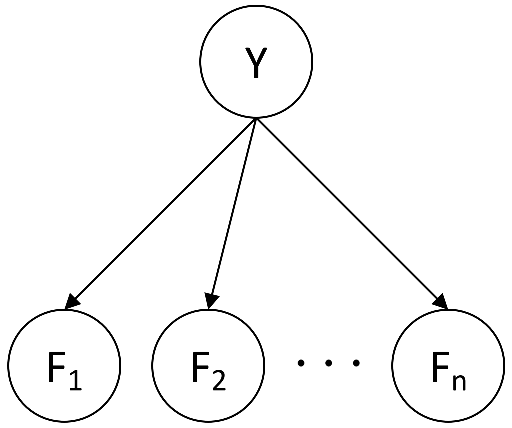
Naïve Bayes Model

- Random variables in this Bayes' net:
  - Y = The label
  - $F_1, F_2, \ldots, F_n$ = The n features
- Probability tables in this Bayes' net:
  - $P(Y)$ = Probability of each label occurring, given no information about the features. Sometimes called the *prior*.
  - $P(F_i|Y)$ = One table per feature. Probability distribution over a feature, given the label.



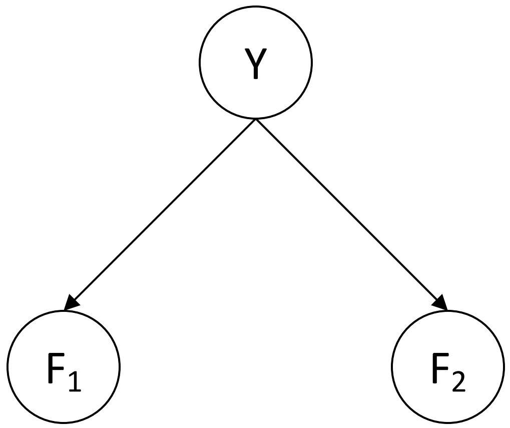
Naïve Bayes Model

- To perform training:
  - Use the training dataset to estimate the probability tables.
  - Estimate $P(Y)$ = how often does each label occur?
  - Estimate $P(F_i|Y)$ = how does the label affect the feature?
- To perform classification:
  - Instantiate all features. You know the input features, so they're your evidence.
  - Query for $P(Y|f_1, f_2, \ldots, f_n)$. Probability of label, given all the input features. Use an inference algorithm (e.g. variable elimination) to compute this.



Example: Naïve Bayes for Spam Filter

- Step 1: Select a ML algorithm. We choose to model the problem with Naïve Bayes.
- Step 2: Choose features to use.



Y: The label (spam or ham)	
Y	P(Y)
ham	?
spam	?

F_1: A feature (do I know the sender?)		
F_1	Y	$P(F_1 \mid Y)$
yes	ham	?
no	ham	?
yes	spam	?
no	spam	?

F_2: Another feature (# of occurrences of FREE)		
F_2	Y	$P(F_2 \mid Y)$
0	ham	?
1	ham	?
2	ham	?
0	spam	?
1	spam	?
2	spam	?

Example: Naïve Bayes for Spam Filter

- Step 3: Training: Use training data to fill in the probability tables.

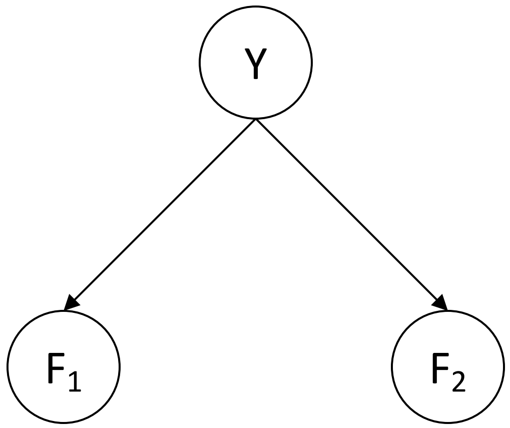
F_2: # of occurrences of FREE		
F_2	Y	$P(F_2 \mid Y)$
0	ham	0.5
1	ham	0.5
2	ham	0.0
0	spam	0.25
1	spam	0.50
2	spam	0.25

Training Data		
#	Email Text	Label
1	Attached is my portfolio.	ham
2	Are you **free** for a meeting tomorrow?	ham
3	**Free** unlimited credit cards!!!!	spam
4	Mail $10,000 check to this address	spam
5	Sign up now for 1 **free** Bitcoin	spam
6	**Free** money **free** money	spam

Row 4: $P(F_2=0 \mid Y=\text{spam}) = 0.25$ because 1 out of 4 spam emails contains “free” 0 times.
Row 5: $P(F_2=1 \mid Y=\text{spam}) = 0.50$ because 2 out of 4 spam emails contains “free” 1 time.
Row 6: $P(F_2=2 \mid Y=\text{spam}) = 0.25$ because 1 out of 4 spam emails contains “free” 2 times.

Example: Naïve Bayes for Spam Filter

- Model trained on a larger dataset:



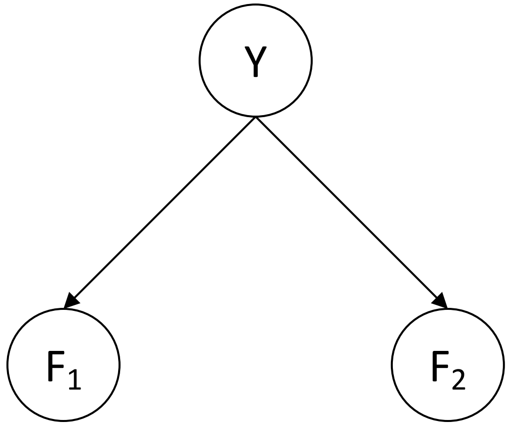
Y: The label (spam or ham)	
Y	P(Y)
ham	0.6
spam	0.4

F_1: A feature (do I know the sender?)		
F_1	Y	$P(F_1\|Y)$
yes	ham	0.7
no	ham	0.3
yes	spam	0.1
no	spam	0.9

F_2: Another feature (# of occurrences of FREE)		
F_2	Y	$P(F_2\|Y)$
0	ham	0.85
1	ham	0.07
2	ham	0.08
0	spam	0.75
1	spam	0.12
2	spam	0.13

Example: Naïve Bayes for Spam Filter

- Step 4: Classification
- Suppose you want to label this email from a known sender:
  "**Free** food in Soda 430 today"
- Step 4.1: Feature extraction:
  - F_1 = yes, known sender
  - F_2 = 1 occurrence of "free"



Example: Naïve Bayes for Spam Filter

- Step 4.2: Inference
- Instantiate features (evidence):
  - F_1 = yes
  - F_2 = 1
- Compute joint probabilities:
  - $P(Y = \text{spam}, F_1 = \text{yes}, F_2 = 1) = P(Y = \text{spam})\ P(F_1 = \text{yes} \mid \text{spam})\ P(F_2 = 1 \mid \text{spam})$
    $= 0.4 * 0.1 * 0.12 = 0.0048$
  - $P(Y = \text{ham}, F_1 = \text{yes}, F_2 = 1) = P(Y = \text{ham})\ P(F_1 = \text{yes} \mid \text{ham})\ P(F_2 = 1 \mid \text{ham})$
    $= 0.6 * 0.7 * 0.07 = 0.0294$
- Normalize:
  - $P(Y = \text{spam} \mid F_1 = \text{yes}, F_2 = 1) = 0.0048 / (0.0048+0.0294) = 0.14$
  - $P(Y = \text{ham} \mid F_1 = \text{yes}, F_2 = 1) = 0.0294 / (0.0048+0.0294) = 0.86$
- Classification result:
  - 14% chance the email is spam. 86% chance it's ham.
  - Or, if you don't need probabilities, note that 0.0294 > 0.0048 and guess ham.

Y: The label (spam or ham)	
Y	P(Y)
ham	0.6
spam	0.4

F_1: do I know the sender?		
F_1	Y	$P(F_1 \mid Y)$
yes	ham	0.7
no	ham	0.3
yes	spam	0.1
no	spam	0.9

F_2: # of occurrences of FREE		
F_2	Y	$P(F_2 \mid Y)$
0	ham	0.85
1	ham	0.07
2	ham	0.08
0	spam	0.75
1	spam	0.12
2	spam	0.13

General Naïve Bayes

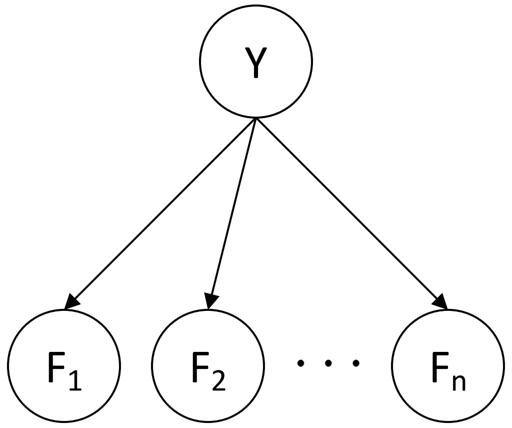
- A general Naive Bayes model:

|Y| parameters

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

$|Y| \times |F|^n$ 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

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

$$\frac{}{P(f_1 \dots f_n)} \quad +$$

$$\Downarrow$$

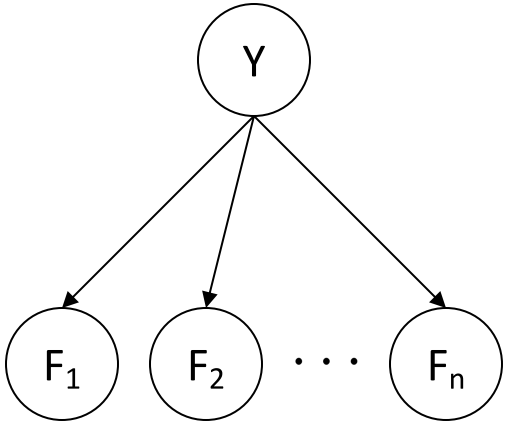
$$P(Y|f_1 \dots f_n)$$

  - Step 2: sum to get probability of evidence

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

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

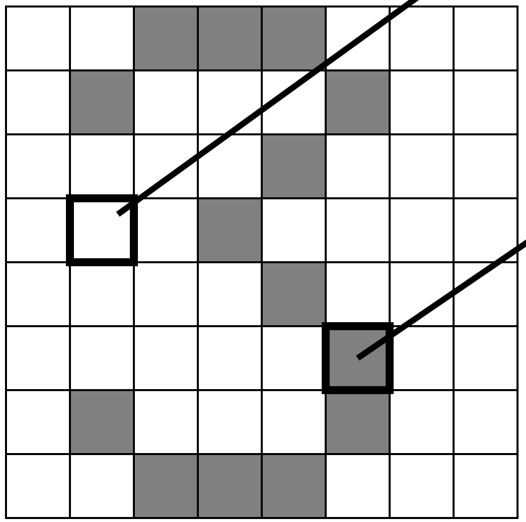
- Naïve Bayes model: $P(Y|F_{0,0} \ldots F_{15,15}) \propto P(Y) \prod_{i,j} P(F_{i,j}|Y)$

- 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

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

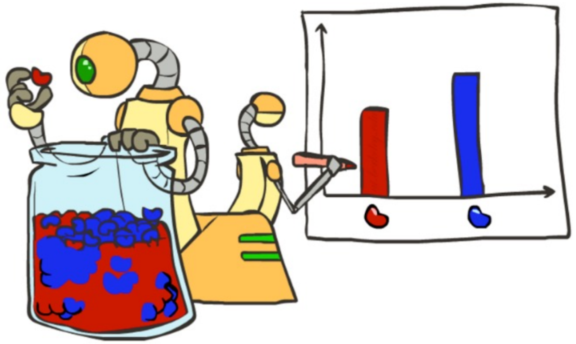
1	0.05
2	0.01
3	0.90
4	0.80
5	0.90
6	0.90
7	0.25
8	0.85
9	0.60
0	0.80

General Naïve Bayes

- 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



- Estimating the distribution of a random variable
- *Elicitation:* ask a human (why is this hard?)
- *Empirically:* use training data (learning!)
  - Example: The parameter θ is the true fraction of red beans in the jar. You don't know θ but would like to estimate it.
  - Collecting training data: You randomly pull out 3 beans:

    r r b

  - Estimating θ using counts, you guess 2/3 of beans in the jar are red.
  - Can we mathematically show that using counts is the "right" way to estimate θ?

Parameter Estimation with Maximum Likelihood

- Can we mathematically show that using counts is the "right" way to estimate θ?
- Maximum likelihood estimation: Choose the θ value that maximizes the probability of the observation
  - In other words, choose the θ value that maximizes P(observation | θ)
  - For our problem:

    P(observation | θ)

    = P(randomly selected 2 red and 1 blue | θ of beans are red)

    = P(red | θ) P(red | θ) P(blue | θ)

    = $\theta^2 (1-\theta)$

  - We want to compute:

    $\underset{\theta}{\operatorname{argmax}}\ \theta^2 (1-\theta)$

Parameter Estimation with Maximum Likelihood

- We want to compute:

  $$\underset{\theta}{\text{argmax}}\ \theta^2 (1-\theta)$$

- Set derivative to 0, and solve!
  - Common issue: The likelihood (expression we're maxing) is the product of a lot of probabilities. This can lead to complicated derivatives.
  - Solution: Maximize the log-likelihood instead. Useful fact:

    $$\underset{\theta}{\text{argmax}}\ f(\theta) = \underset{\theta}{\text{argmax}}\ \ln f(\theta)$$

Parameter Estimation with Maximum Likelihood

$\underset{\theta}{\operatorname{argmax}}\, \theta^2(1-\theta)$	Find θ that maximizes likelihood
$= \underset{\theta}{\operatorname{argmax}} \ln\left(\theta^2(1-\theta)\right)$	Find θ that maximizes log-likelihood (will be the same θ)
$\frac{d}{d\theta} \ln\left(\theta^2(1-\theta)\right) = 0$	Set derivative to 0
$\frac{d}{d\theta}\left[\ln(\theta^2) + \ln(1-\theta)\right] = 0$	Logarithm rule: products become sums
$\frac{d}{d\theta}\left[2\ln(\theta) + \ln(1-\theta)\right] = 0$	Logarithm rule: exponentiation becomes multiplication
$\frac{d}{d\theta} 2\ln(\theta) + \frac{d}{d\theta}\ln(1-\theta) = 0$	Now we can derive each term of the original product separately
$\frac{2}{\theta} - \frac{1}{1-\theta} = 0$	Reminder: Derivative of ln(θ) is 1/θ
$\theta = \frac{2}{3}$	Use algebra to solve for θ. If we used arbitrary red and blue counts r and b instead of r=2 and b=1, we'd get θ = r / (r+b), the count estimate.

Maximum Likelihood?

- Relative frequencies are the maximum likelihood estimates

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

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

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

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

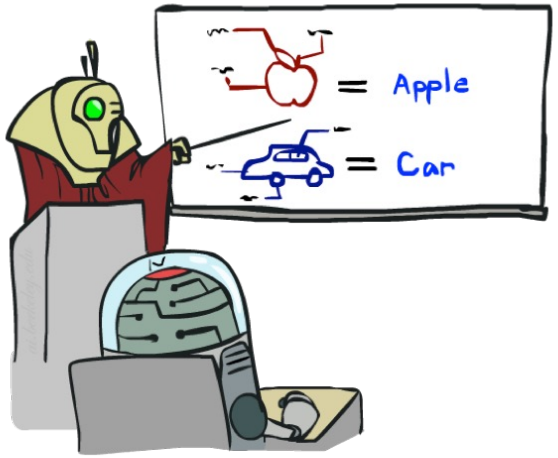
Parameter Estimation with Maximum Likelihood

- 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..

Important Concepts

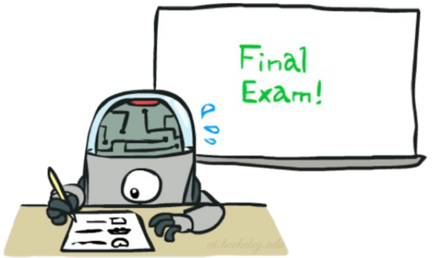
- Data: labeled instances, e.g. emails marked spam/ham
  - Training set
  - Held out set (sometimes also called test or validation set)
  - Test/Independent set
- Features: attribute-value pairs which characterize each x
- Experimentation cycle
  - Learn parameters (e.g. model probabilities) on training 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 (confusion matrix)
  - Many measures out there
- 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

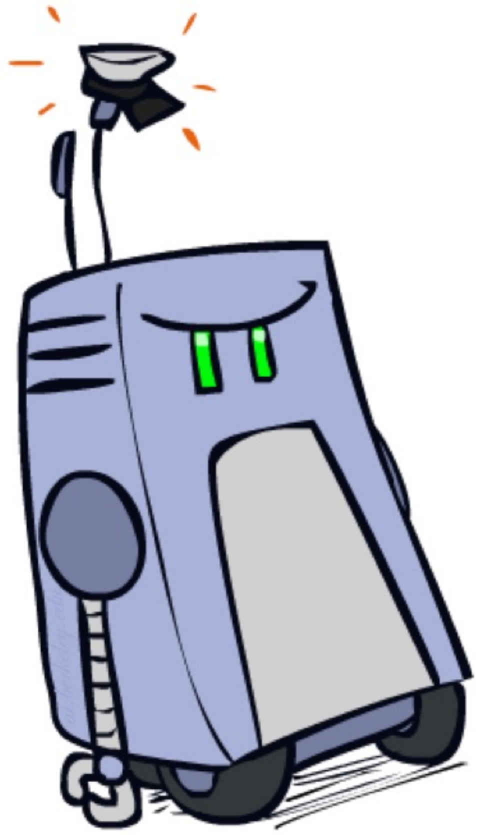


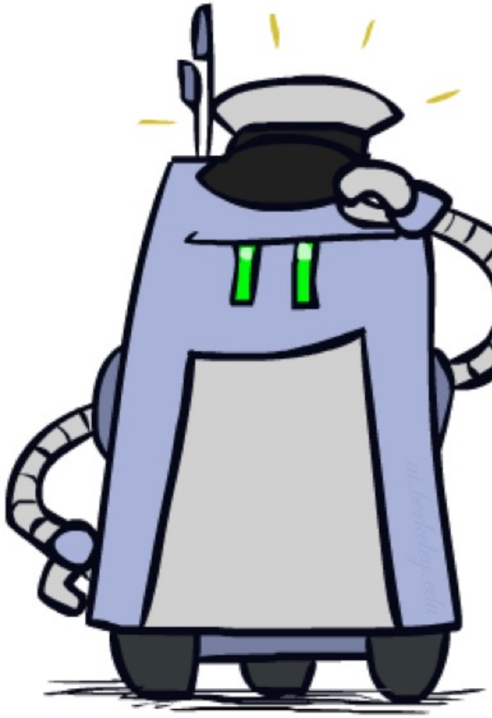
Held-Out Data

Independent Data



Underfitting and Overfitting





Example: Overfitting

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

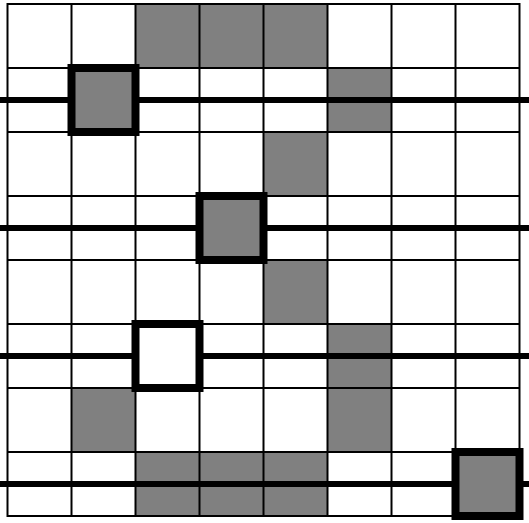
$P(C = 2) = 0.1$

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

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

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

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



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

$P(C = 3) = 0.1$

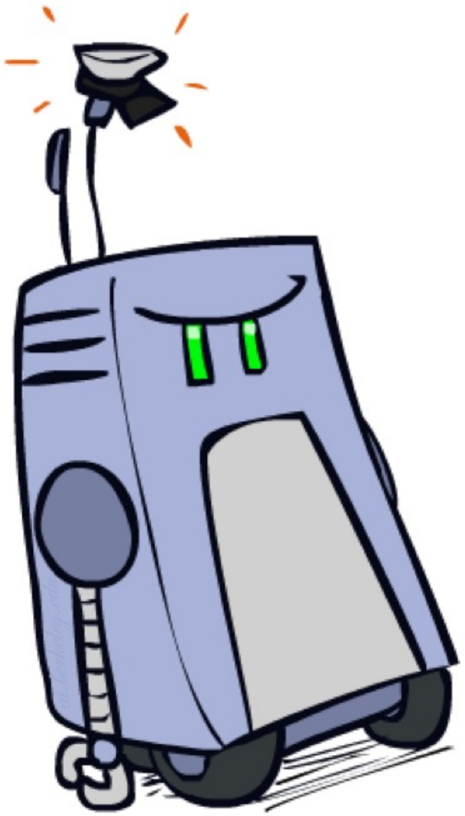
$P(\text{on}|C = 3) = 0.8$

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

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

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

2 wins!!



Example: Overfitting

- *relative* probabilities (odds ratios):

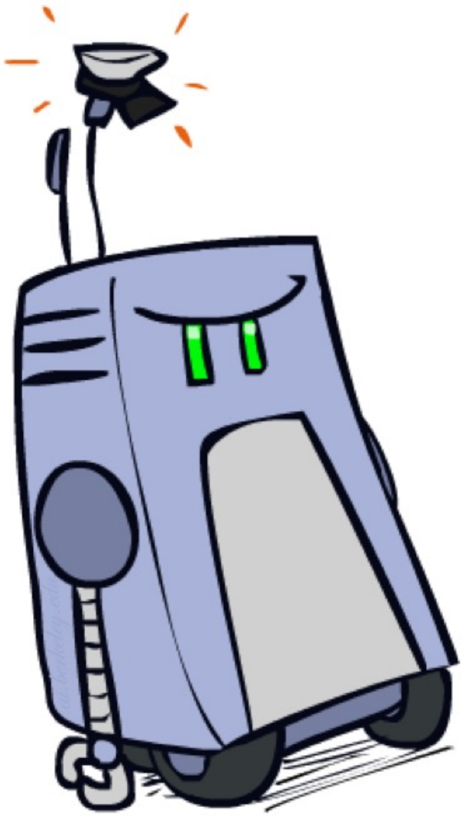
$$\frac{P(W|\text{ham})}{P(W|\text{spam})}$$

```
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?



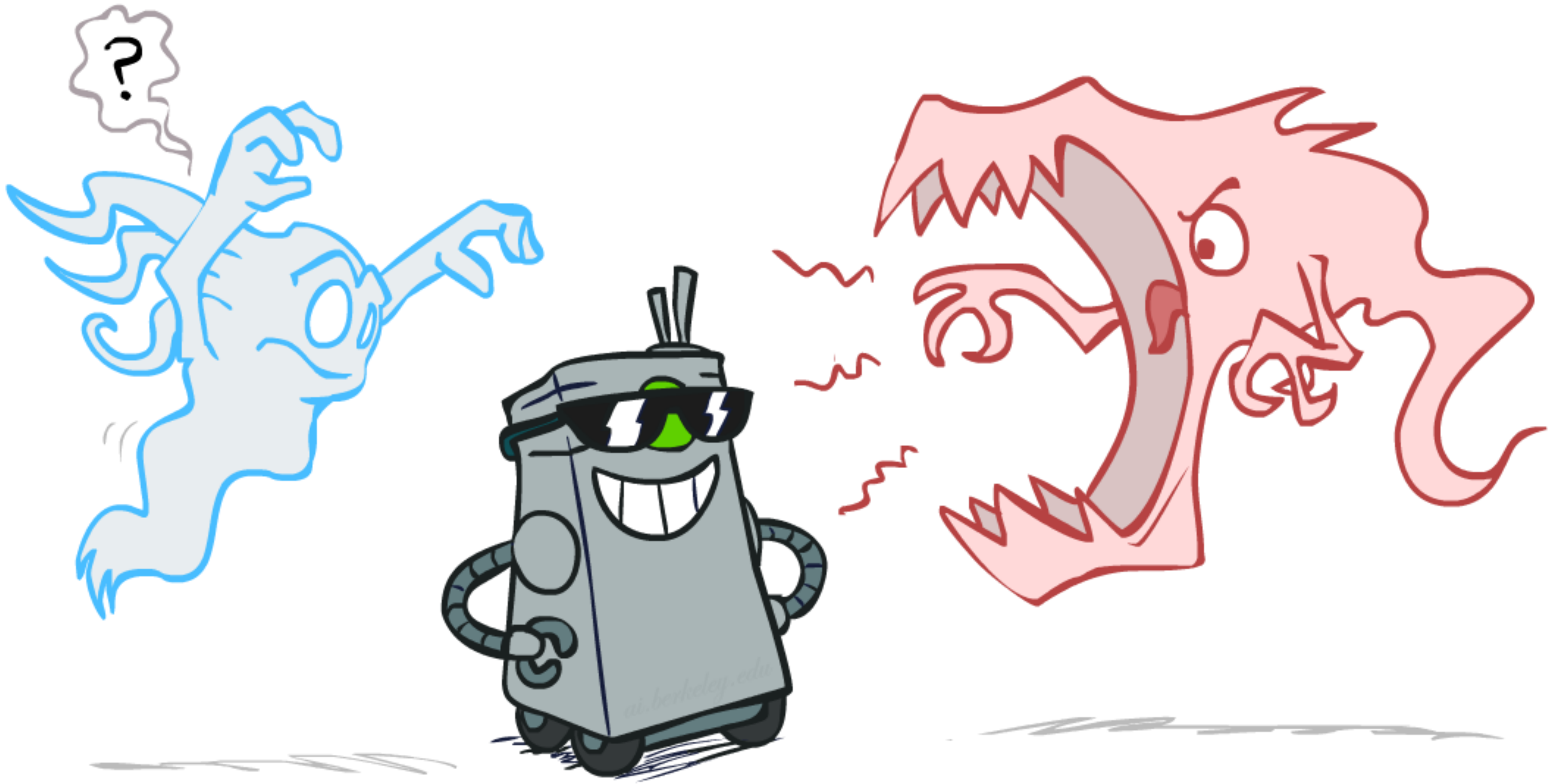
Generalization and Overfitting

- 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

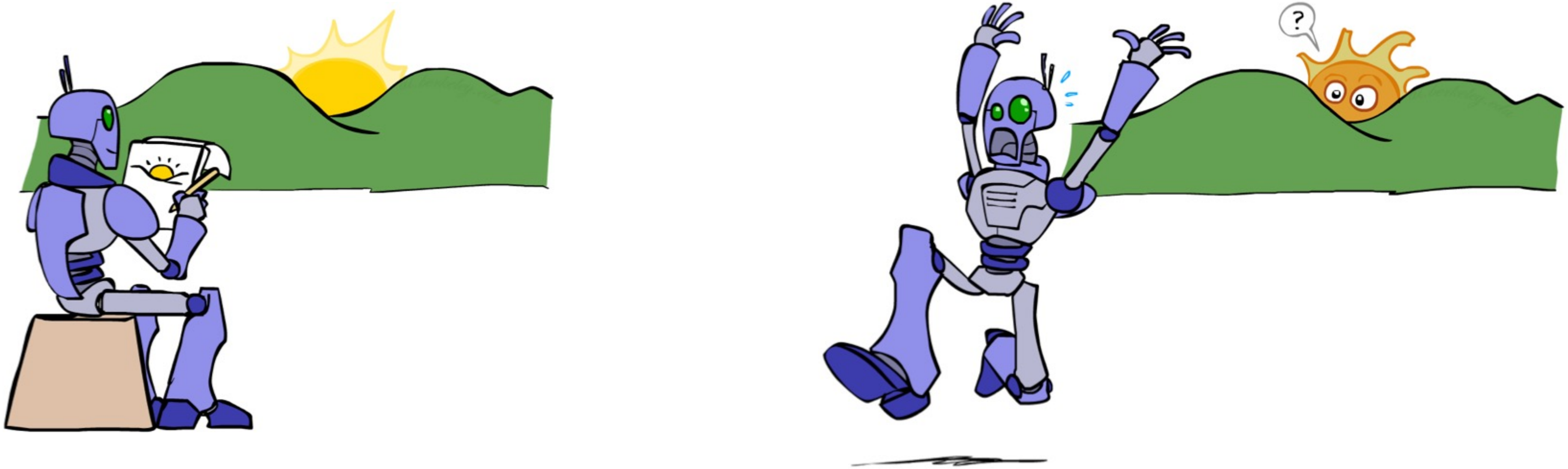
- As an extreme case, imagine using the entire email as the only feature
  - Would get the training data perfect (if deterministic labeling)
  - Wouldn't *generalize* at all
  - Just making the bag-of-words assumption gives us some generalization, but isn't enough

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

Smoothing



Unseen Events



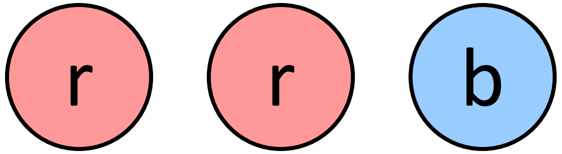
Laplace Smoothing

- 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*



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

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

Laplace Smoothing

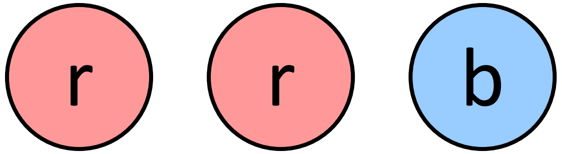
- Laplace's estimate (extended):
  - Pretend you saw every outcome k extra times

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

  - 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

$$\begin{aligned}\theta_{ML} &= \arg\max_{\theta} P(\mathbf{X}|\theta) \\ &= \arg\max_{\theta} \prod_i P_\theta(X_i)\end{aligned} \quad \Rightarrow \quad P_{\text{ML}}(x) = \frac{\text{count}(x)}{\text{total samples}}$$

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

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

"right" choice of P(theta)
-> Laplace estimates

Real NB: Smoothing

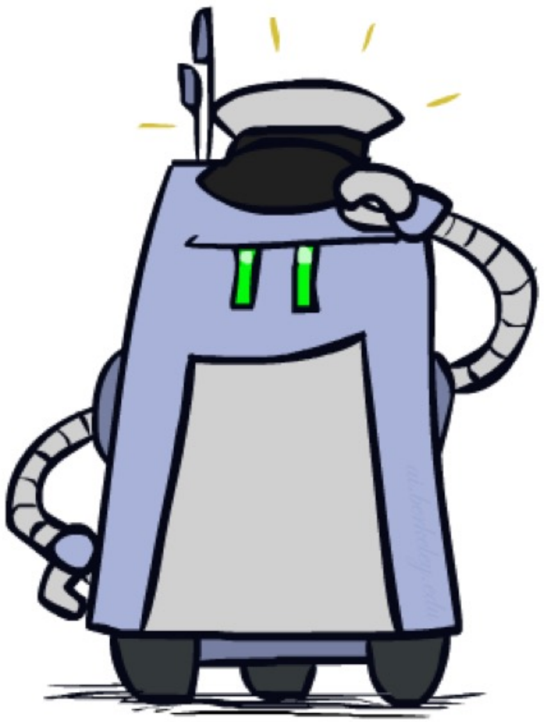
- For real classification problems, smoothing is critical
- New odds ratios:

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

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

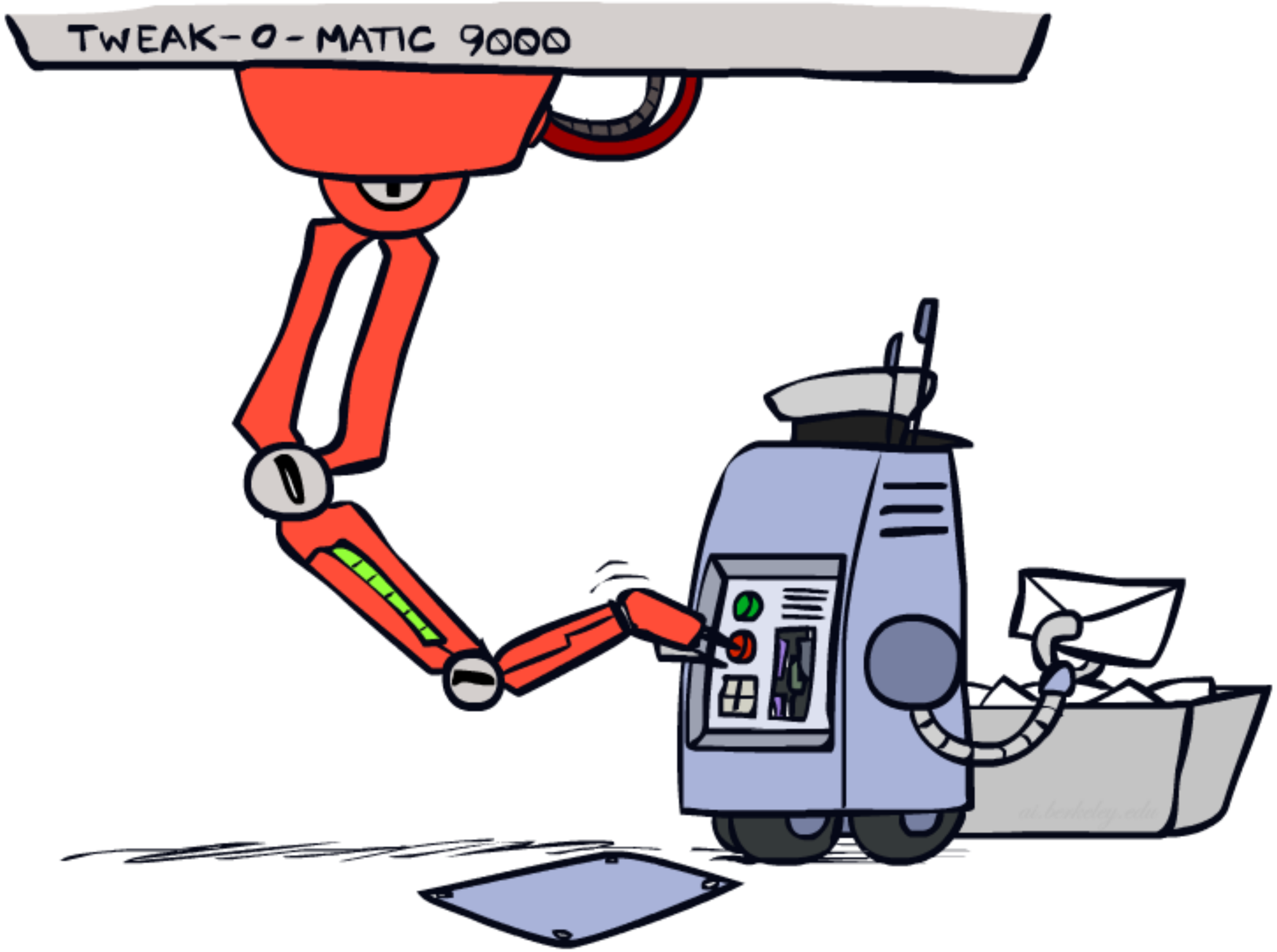
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

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



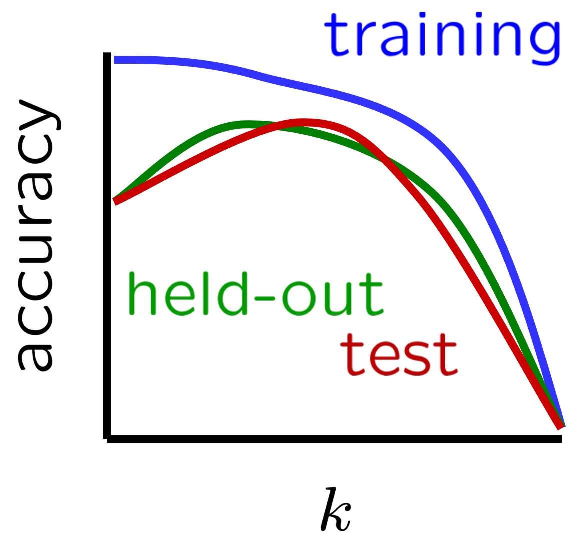
Do these make more sense?

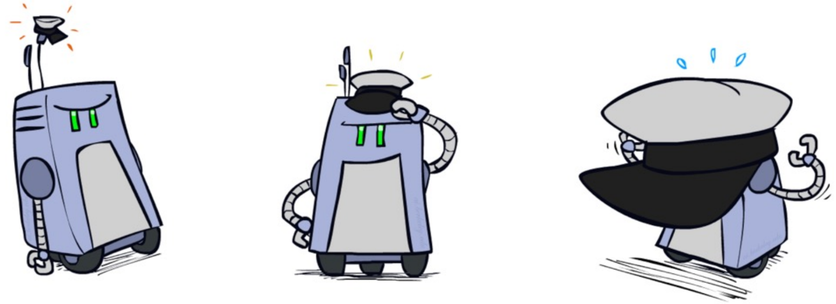
Tuning



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