Ve492: Introduction to Artificial Intelligence

Introduction to Machine Learning

Paul Weng

UM-SJTU Joint Institute

Slides adapted from http://ai.berkeley.edu, AIMA, UM

Today

- Overview of machine learning
- Naïve Bayes
- Common issues encountered in 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)

- Machine learning: techniques that give a computer system the ability to learn to perform a given task
  - Learn = improve itself as it sees more data, observations, interactions

- Machine learning: programming with data

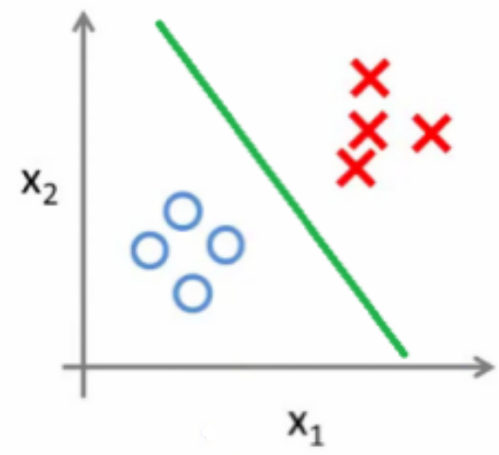
What do we learn from?

Supervised

Label

Classifier
Regressor
Structured predictor

x, y

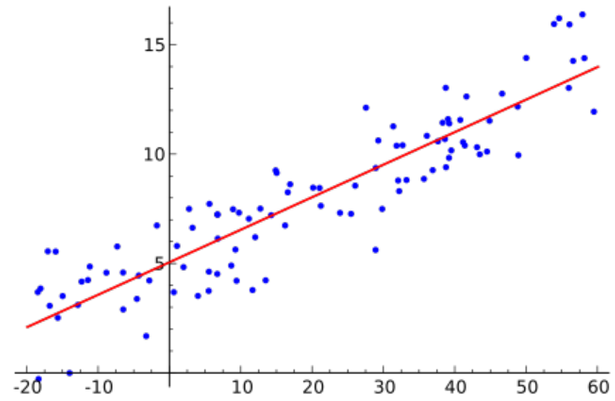


Reinforcement learning
Online learning

Reward

x_t, a_t, r_t, s_{t+1}

Policy



Unsupervised

No feedback

x_i

Latent structure
Hidden concept

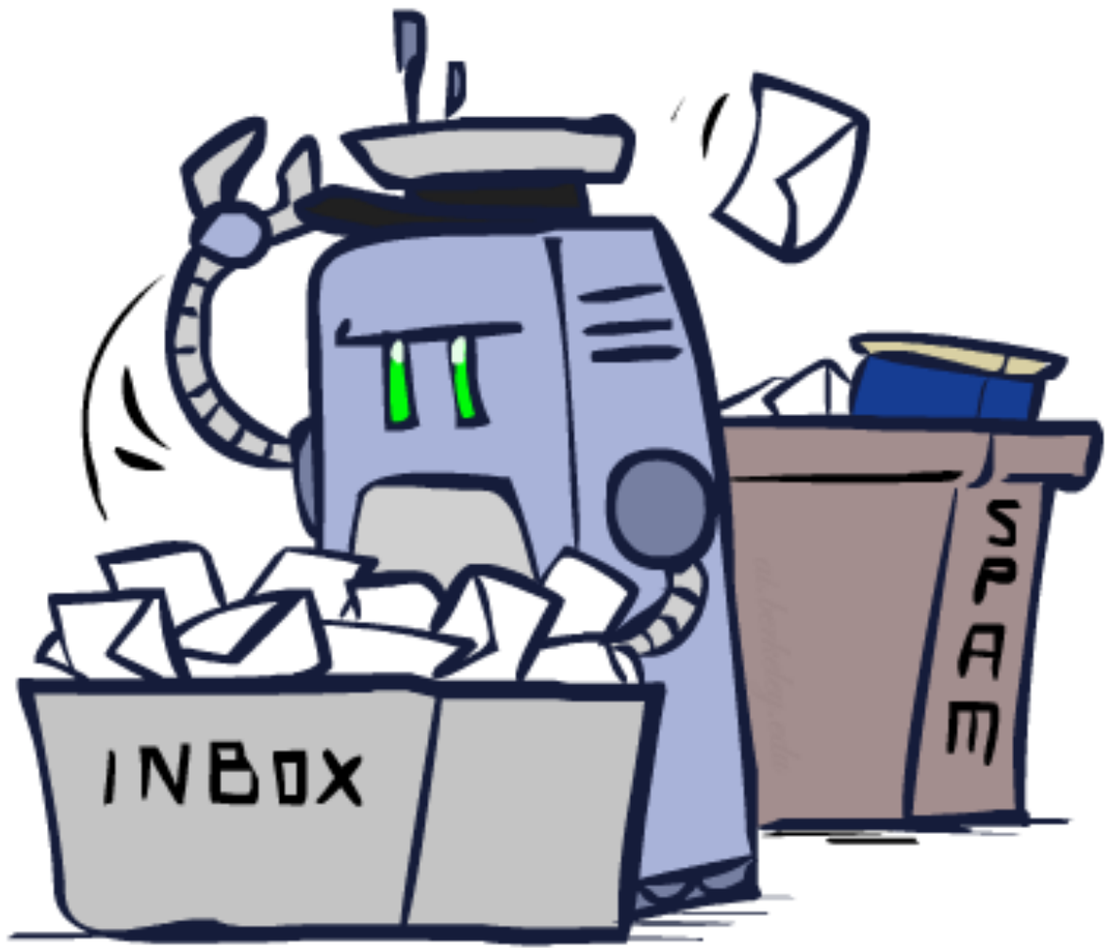
The man at bat readies to swing at the pitch while the umpire looks on.

Typical Supervised ML Pipeline

Data acquisition	Data preprocessing	Feature engineering	Model building, training, selection	Model deployment
Data collection, aggregation, consolidation	Data cleaning, missing data imputation, normalization	Feature construction, selection	**Training** on training dataset, **hyperparameter tuning** on validation dataset, **model selection** on validation dataset, cross-validation, **evaluation** on test dataset	**Profit!**

- Batch vs online settings

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. …

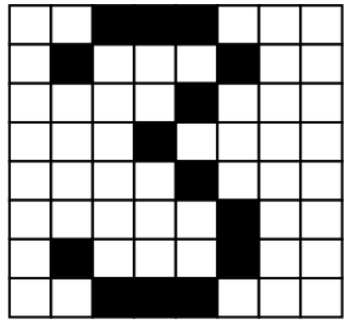
TO BE REMOVED FROM FUTURE MAILINGS, SIMPLY REPLY TO THIS MESSAGE AND PUT "REMOVE" IN THE SUBJECT.

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



0

1

2

1

??

- **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
  - …

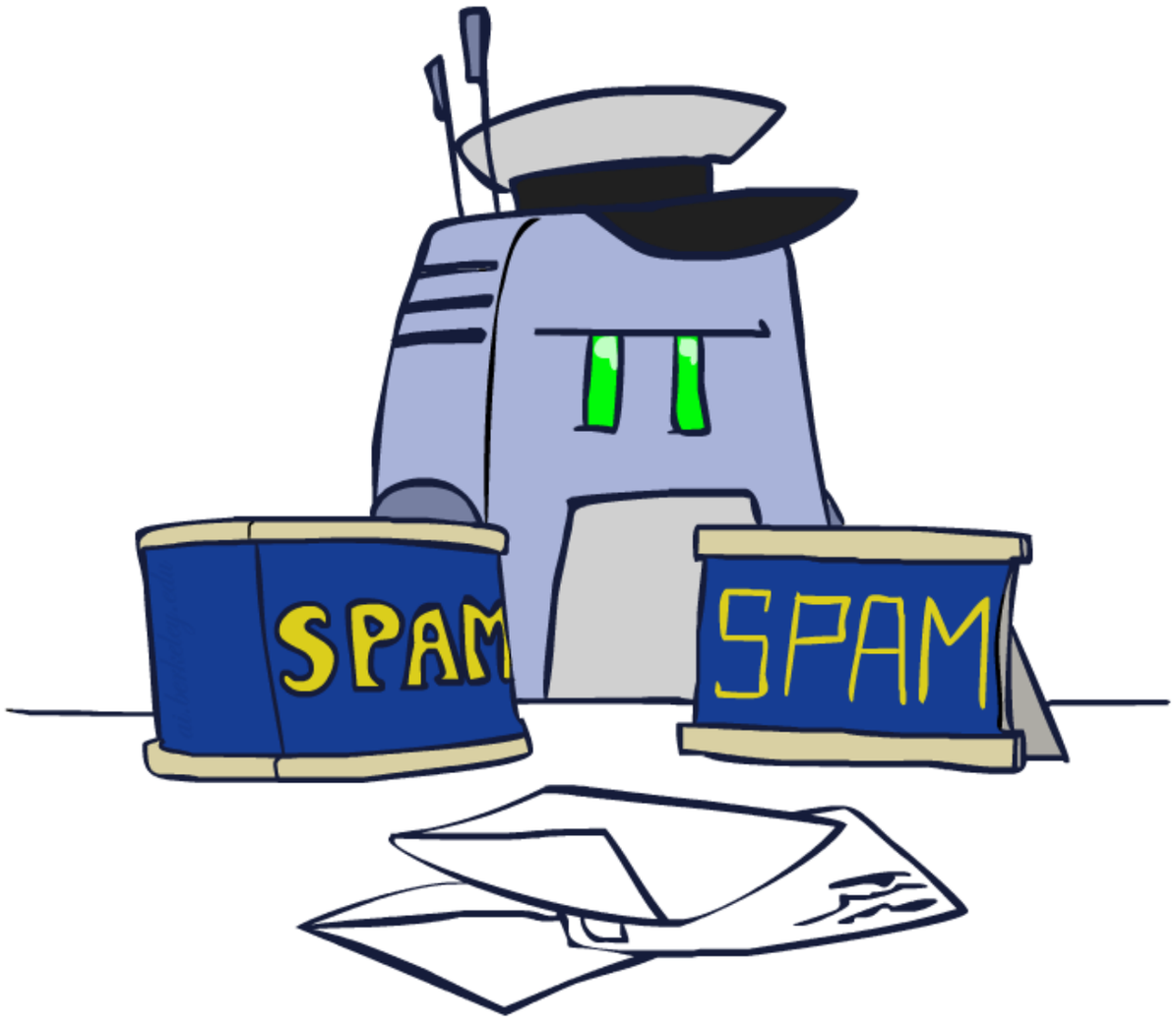
Other Classification Tasks

- 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

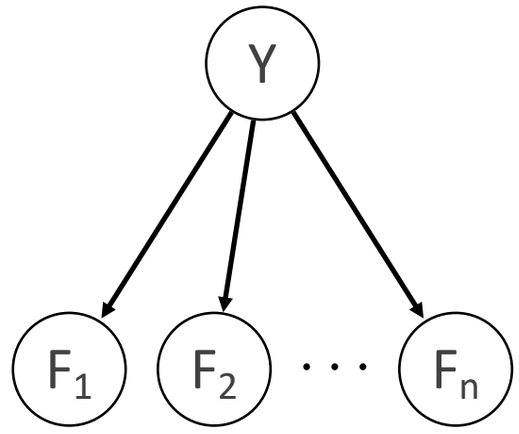
- Model-based approach
  - Build a model (e.g. Bayes' net) where both the label and features are random variables
  - Instantiate any observed features
  - Query for the distribution of the label conditioned on the features

- 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

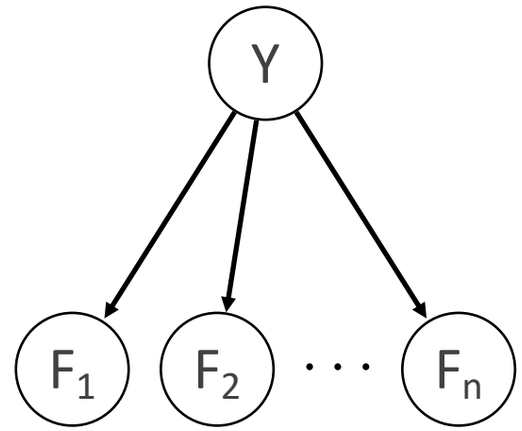
- A general Naive Bayes model:

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

|Y| parameters

|Y| x |F|^n values

n x |F| x |Y| parameters



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

Inference for Naïve Bayes

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

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

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

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

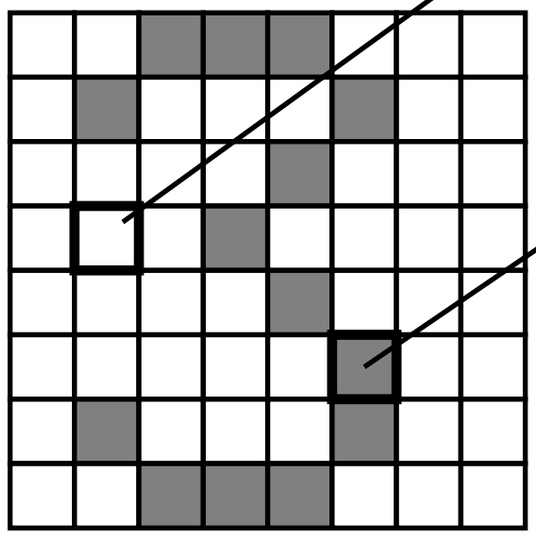
General Naïve Bayes

- What do we need in order to use Naïve Bayes?
  - Inference method (we just saw this part)
    - Start with a bunch of probabilities: $P(Y)$ and the $P(F_i \mid Y)$ tables
    - Use standard inference to compute $P(Y \mid F_1 \ldots F_n)$
    - Nothing new here
  - Estimates of local (conditional) probability tables
    - $P(Y)$, the prior over labels
    - $P(F_i \mid Y)$ 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 were given, 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

Example: 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, validation, test sets

- Classifiers
  - Learn on the training set
  - (Tune it on a validation 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 position i
  - As before: predict label conditioned on feature variables (spam vs. ham)
  - As before: assume features are conditionally independent given label
  - New: each W_i is identically distributed

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

in is lecture lecture next over person remember room sitting the the the to to up wake when you

Example: Spam Filtering

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

$P(Y)$

```
ham : 0.66
spam: 0.33
```

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

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

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

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

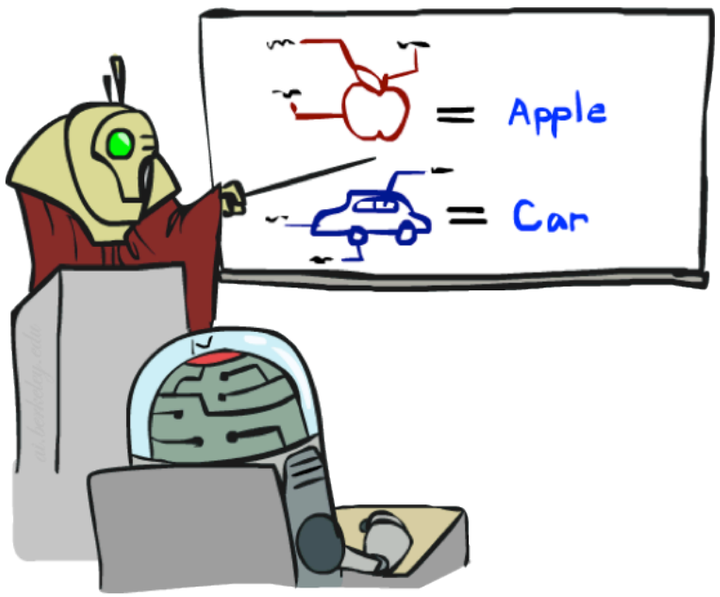
- Where do these tables come from?

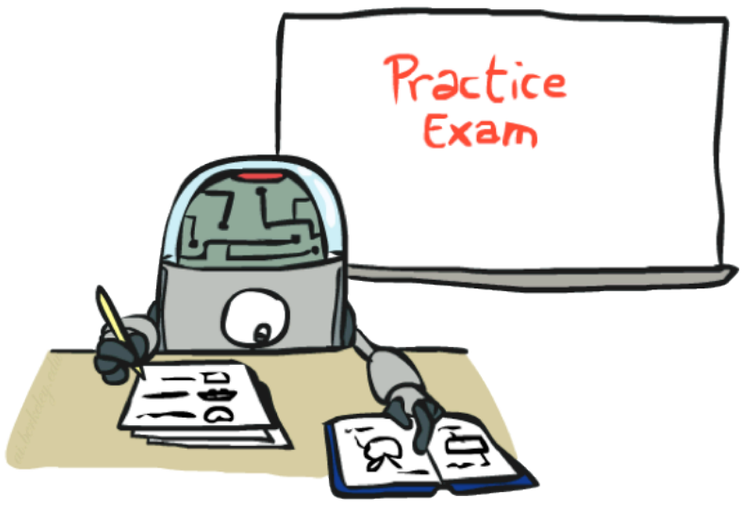
Spam Example

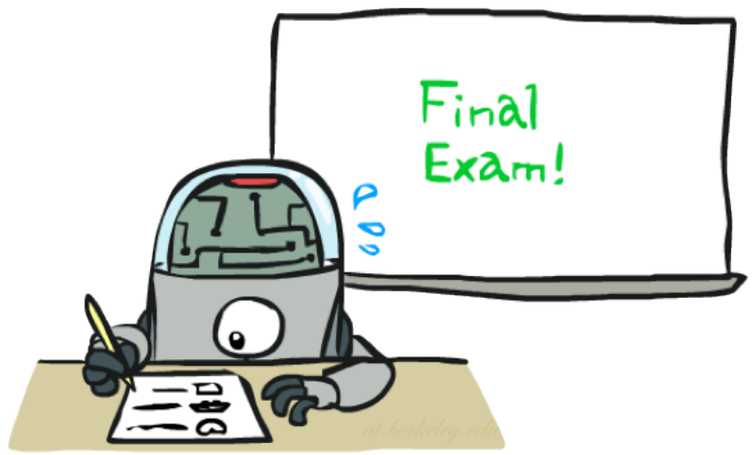
	Word	P(w|spam)	P(w|ham)	Tot Spam	Tot Ham
$P(Y)$	(prior)	0.33333	0.66666	-1.1	-0.4
$P(W_1\|Y)$					
$P(W_2\|Y)$					
⋮					

$$P(\text{spam} \mid w) = 0.989$$

Training and Testing

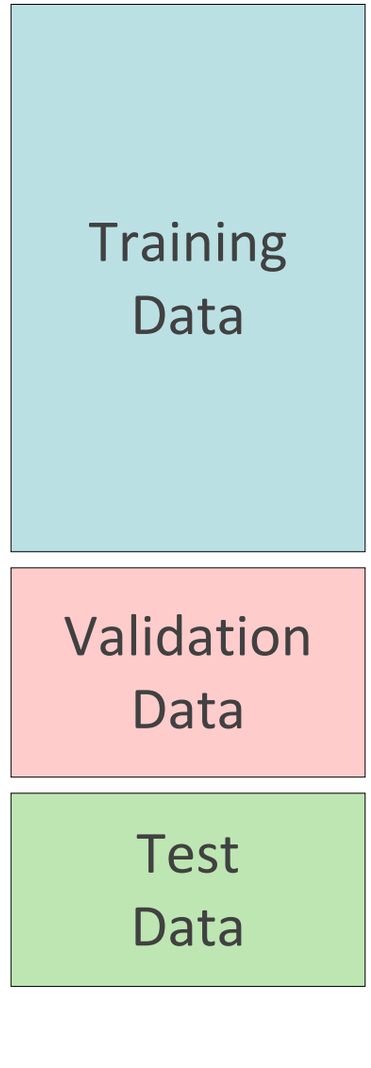




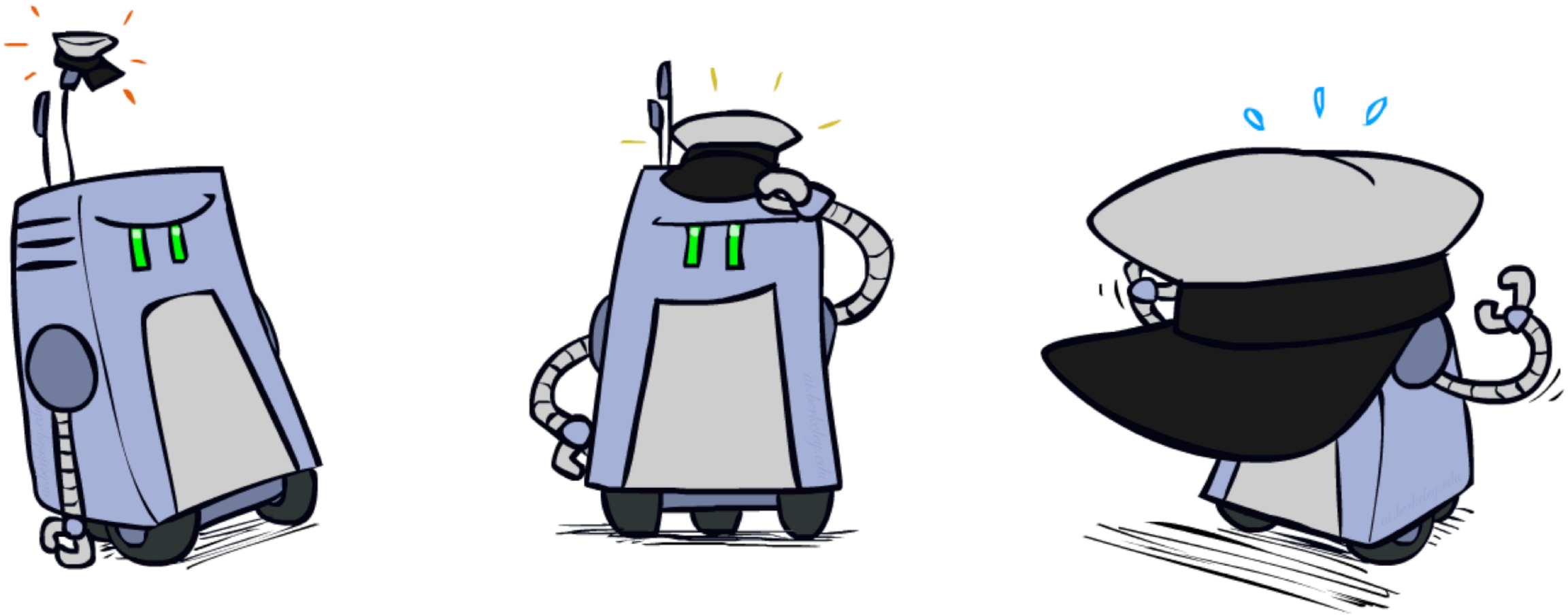


Important Concepts

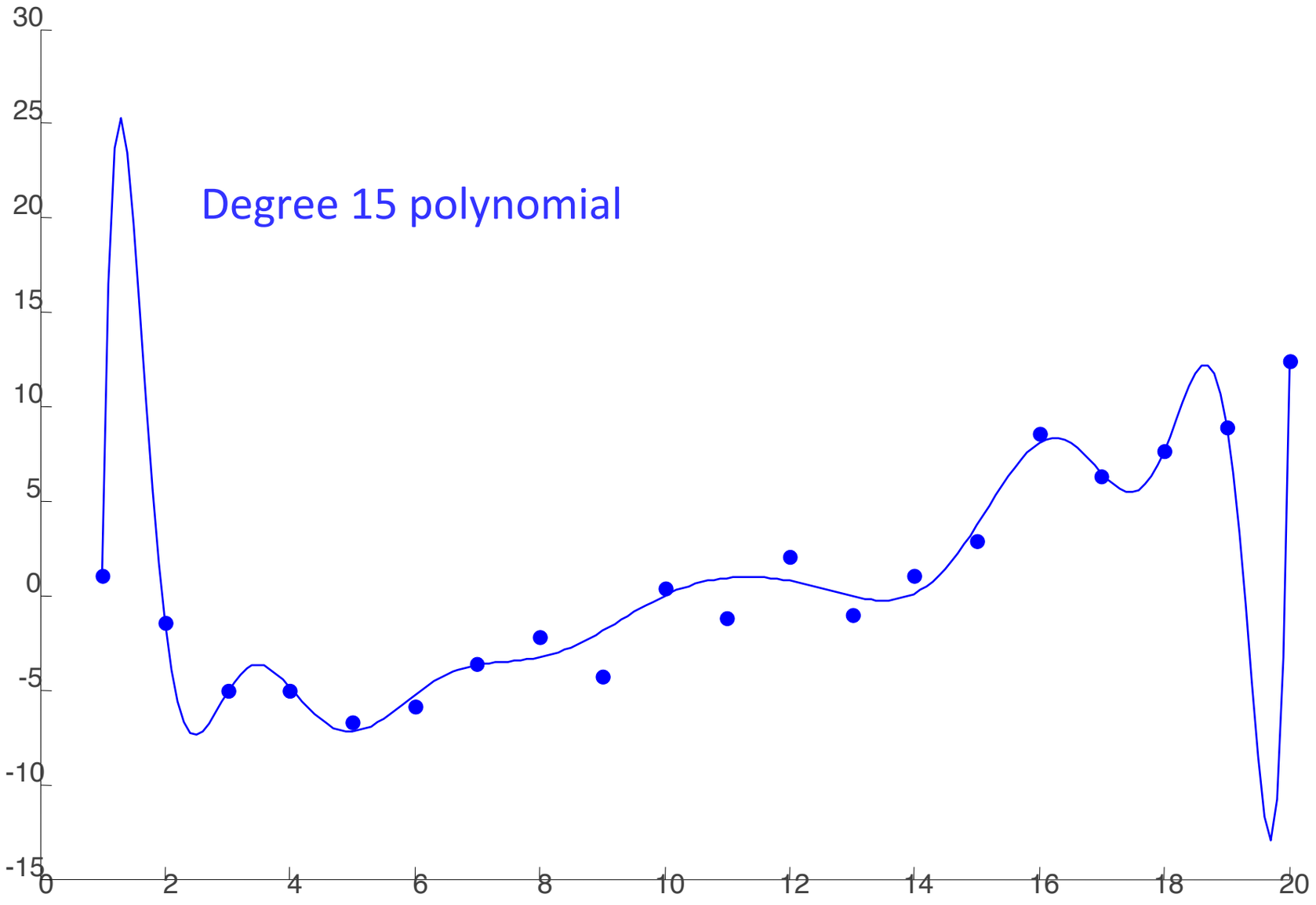
- **Data**: labeled instances, e.g., emails marked spam/ham
  - Training set
  - Validation set
  - Test set
- **Features**: attribute-value pairs which characterize each x
- Experimentation cycle
  - Learn parameters (e.g., model probabilities) on training set
  - (Tune hyperparameters on validation 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
  - **Underfitting**: fits the training set poorly



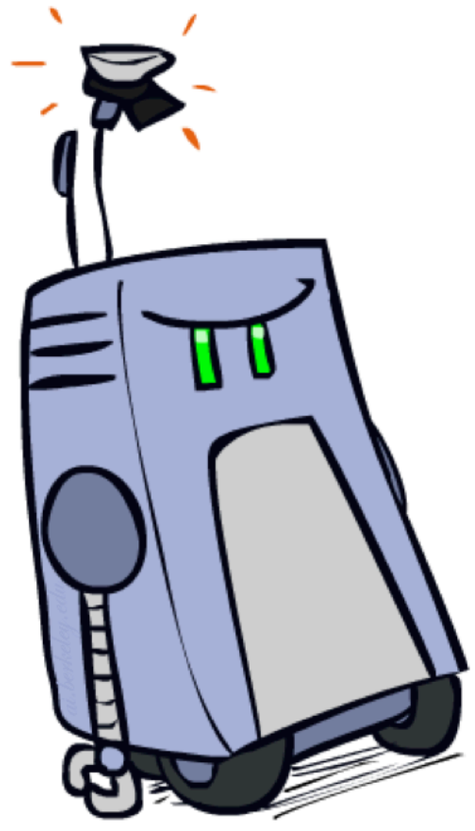
Underfitting and Overfitting



Overfitting



Degree 15 polynomial



Example: Overfitting

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

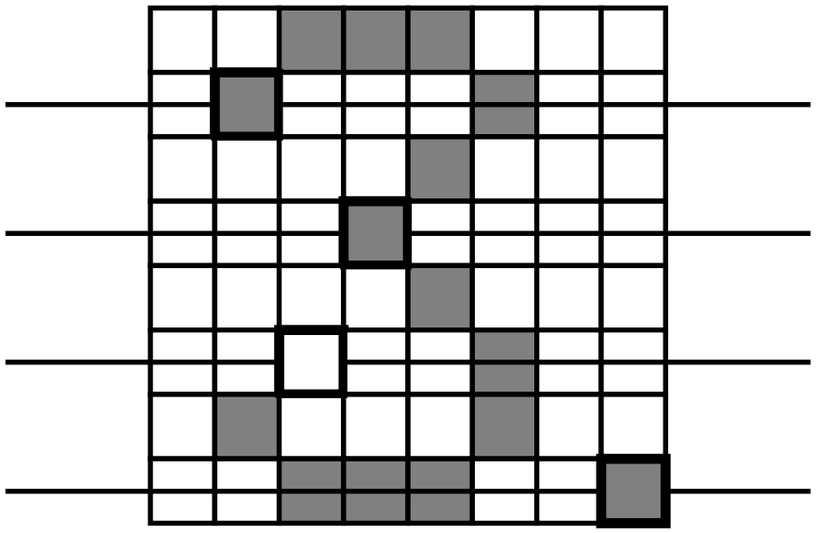
$P(C = 2) = 0.1$

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

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

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

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



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

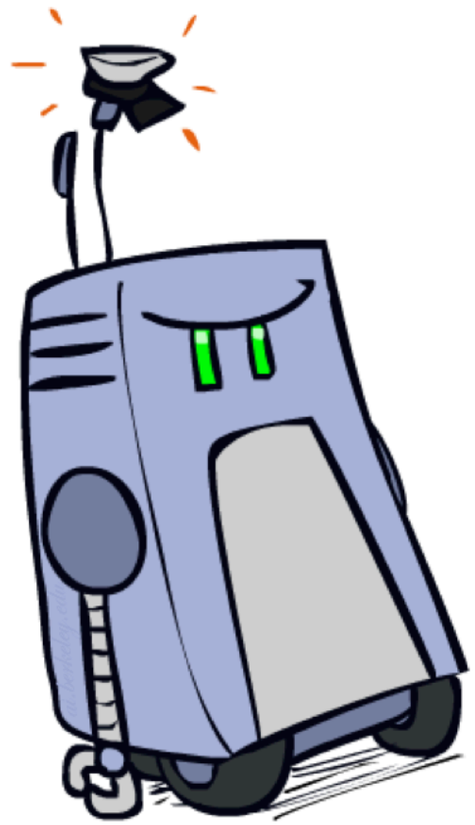
$P(C = 3) = 0.1$

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

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

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

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



2 wins!!

Example: Overfitting

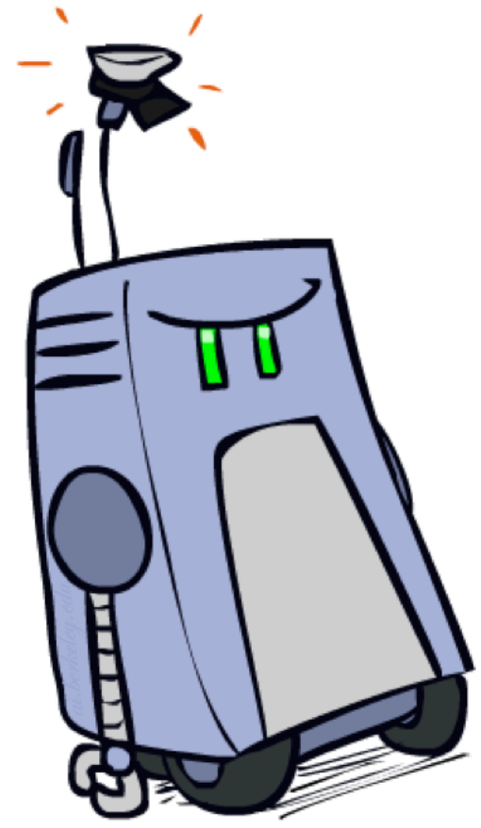
- Posteriors determined by *relative* probabilities (odds ratios):

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

```
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?

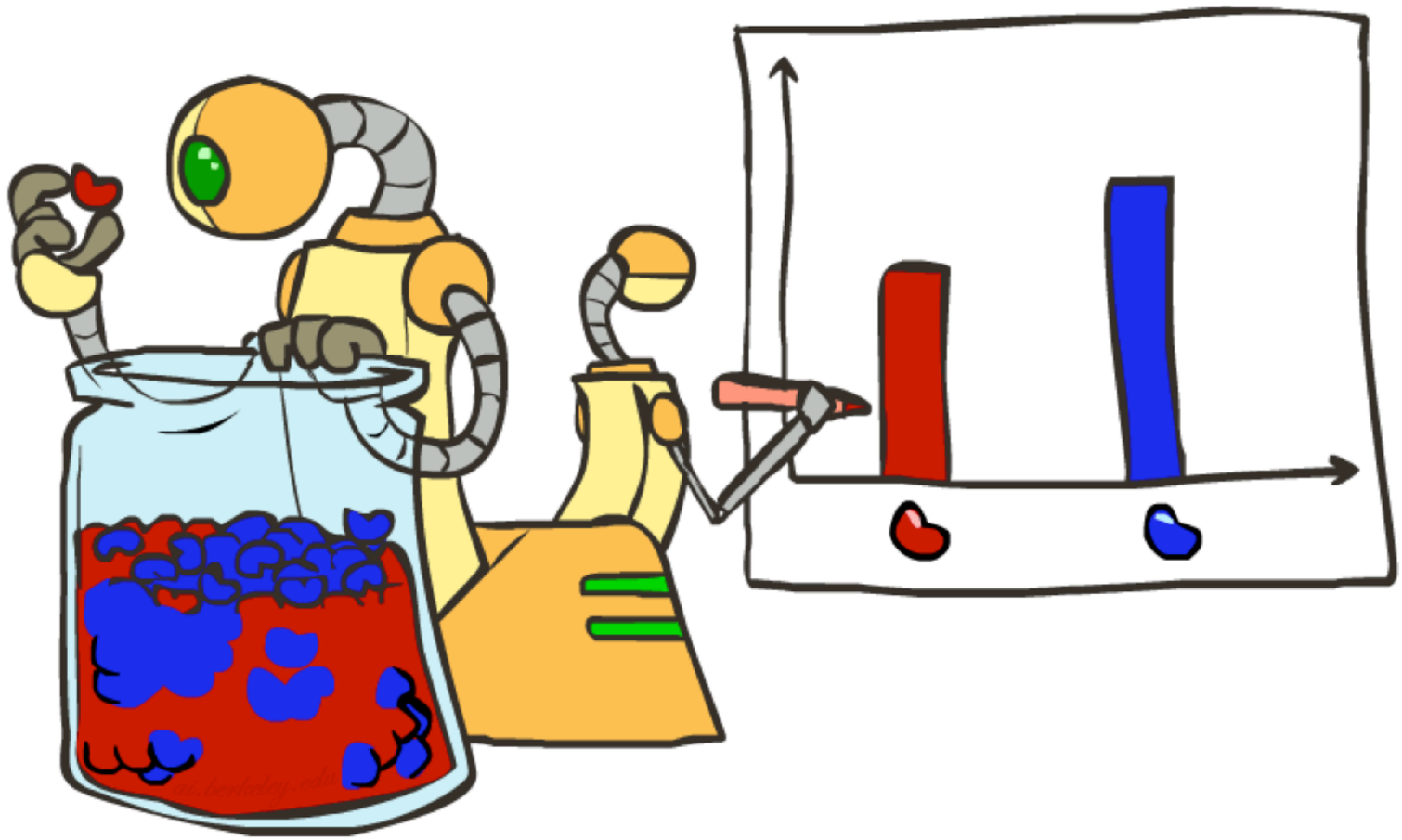
Generalization and Overfitting

- 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

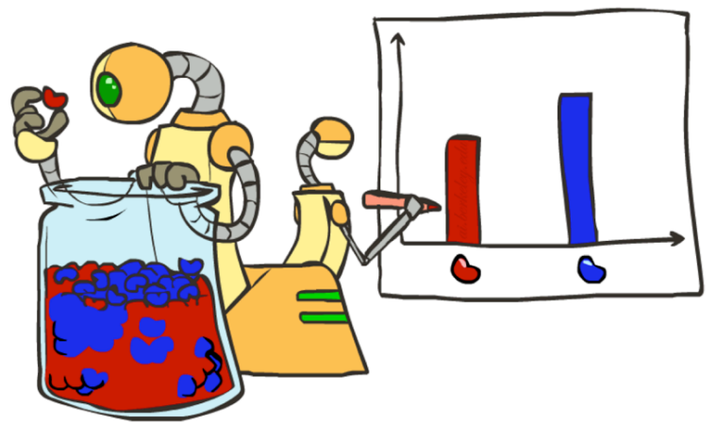
- To generalize better: we need to smooth or regularize the estimates

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:



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

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

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

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

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

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

Maximum Likelihood Estimation

- **Data:** Observed set D of α_H Head and α_T Tail
- **Hypothesis space:** Binomial distributions Bin(θ, $\alpha_H+\alpha_T$)
- **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

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

Maximum Likelihood Estimation

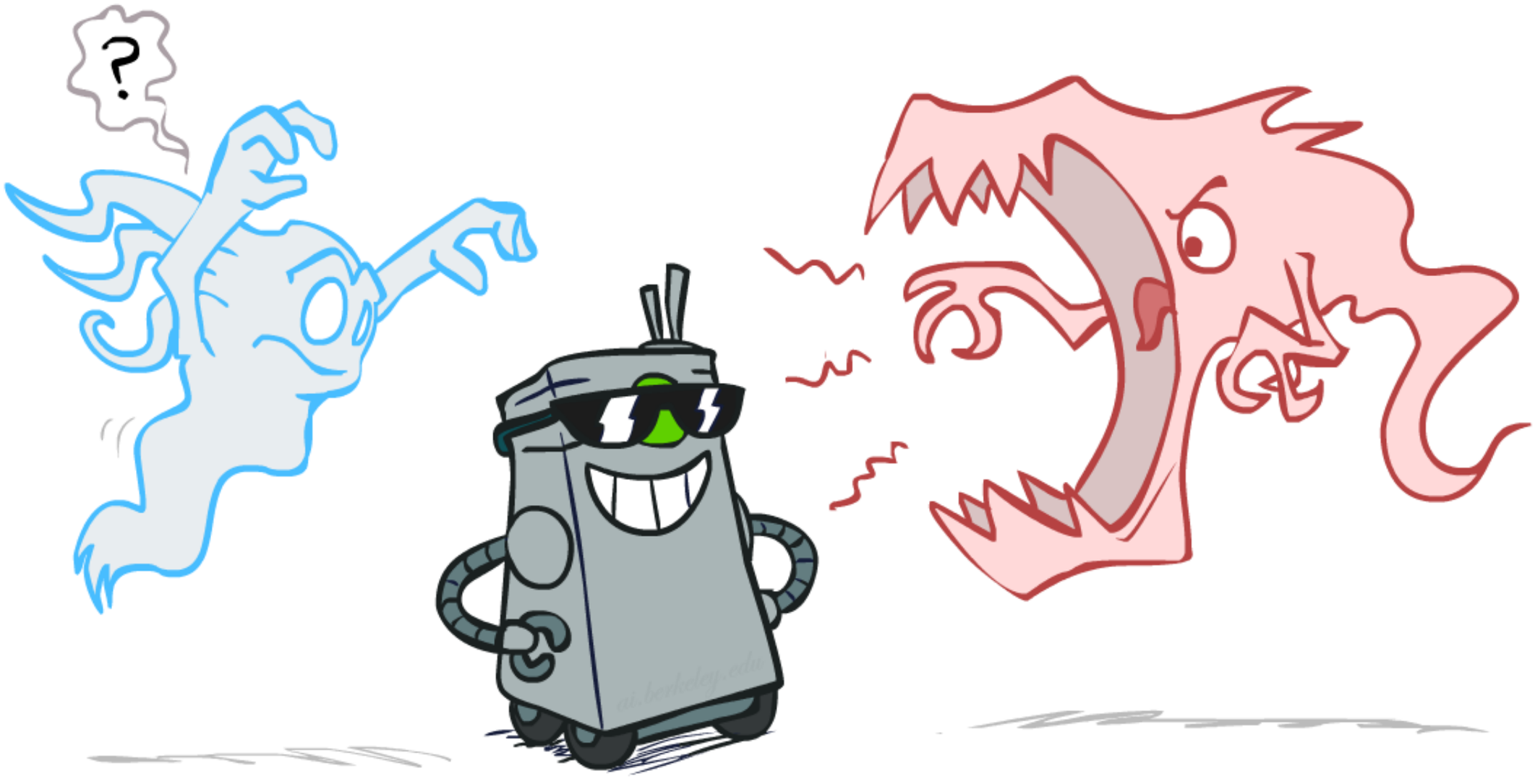
$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} \ln P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\end{aligned}$$

- Set derivative to zero, and solve!

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

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

Smoothing



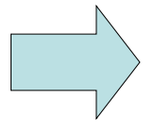
Maximum Likelihood?

- Relative frequencies are the maximum likelihood estimates

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

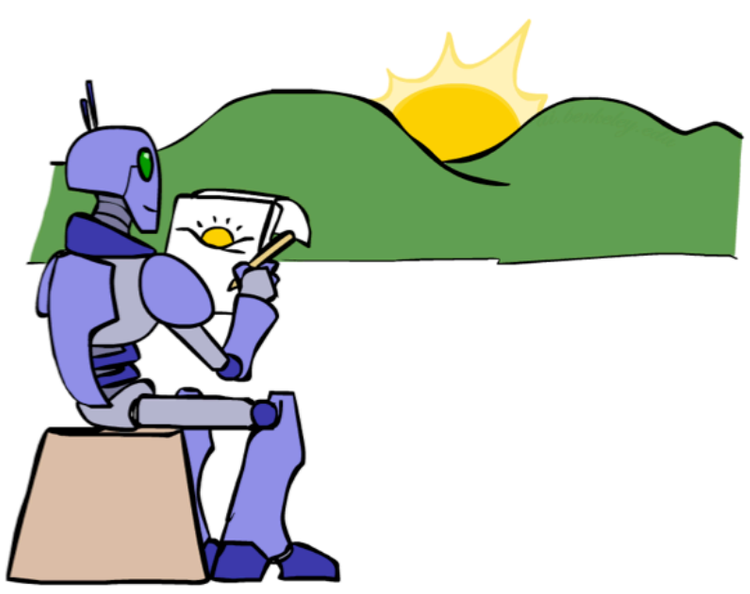
- Another option is to consider the most likely parameter value given the data

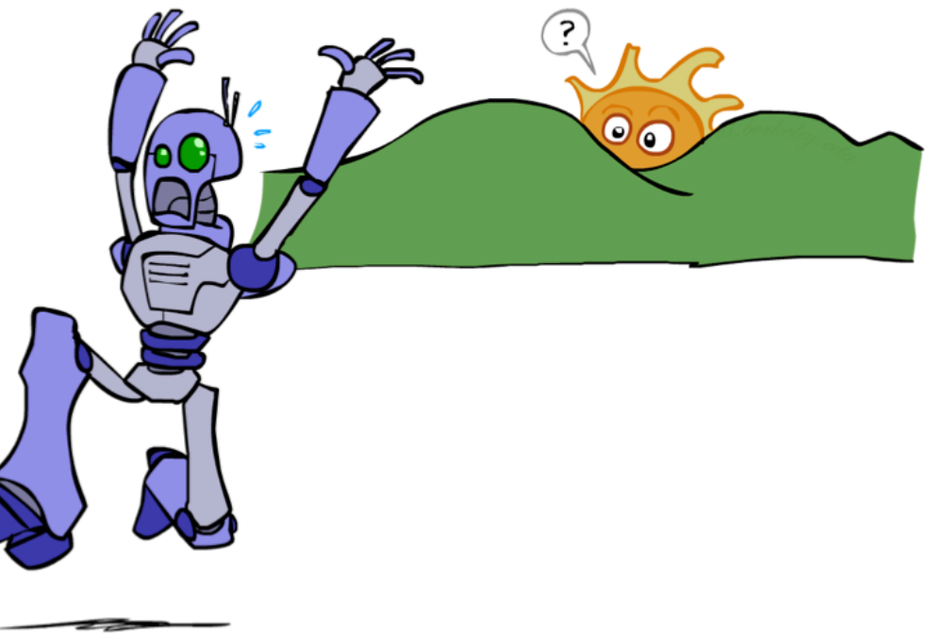
$$\theta_{MAP} = \arg\max_{\theta} P(\theta|\mathbf{X}) = \arg\max_{\theta} P(\mathbf{X}|\theta)P(\theta)/P(\mathbf{X}) = \arg\max_{\theta} P(\mathbf{X}|\theta)P(\theta)$$



????

Unseen Events





Laplace Smoothing

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

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

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

$P_{ML}(X) =$ <2/3,1/3>

- Can derive this estimate with Dirichlet Priors

$P_{LAP}(X) =$ <3/5,2/5>

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

$P_{LAP,0}(X) =$ <2/3,1/3>

- Laplace for conditionals:
  - Smooth each condition independently:

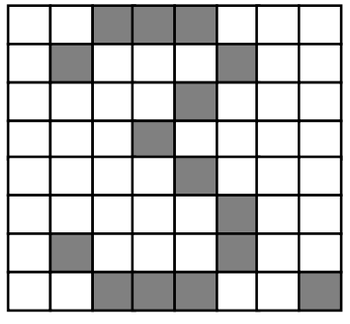
$P_{LAP,1}(X) =$ <3/5,2/5>

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

$P_{LAP,100}(X) =$ <102/203,101/203>

Estimation: Linear Interpolation*

- In practice, Laplace can perform 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?

Real NB: Smoothing

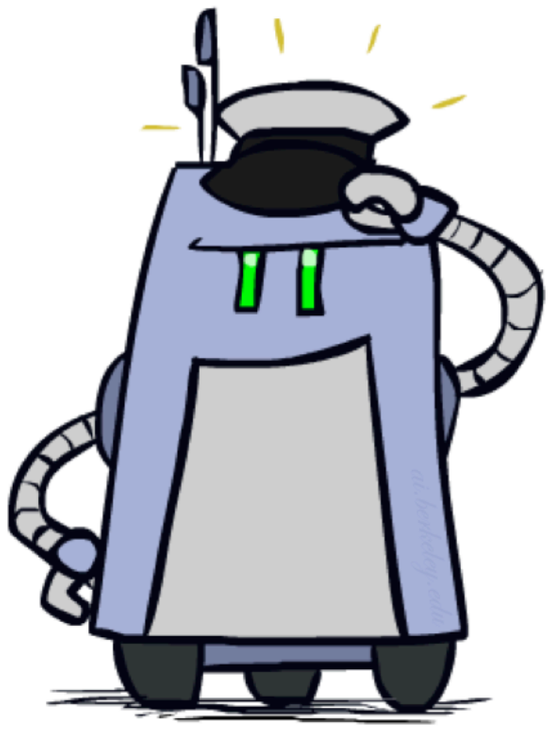
- For real classification problems, smoothing is critical
- New odds ratios:

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

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

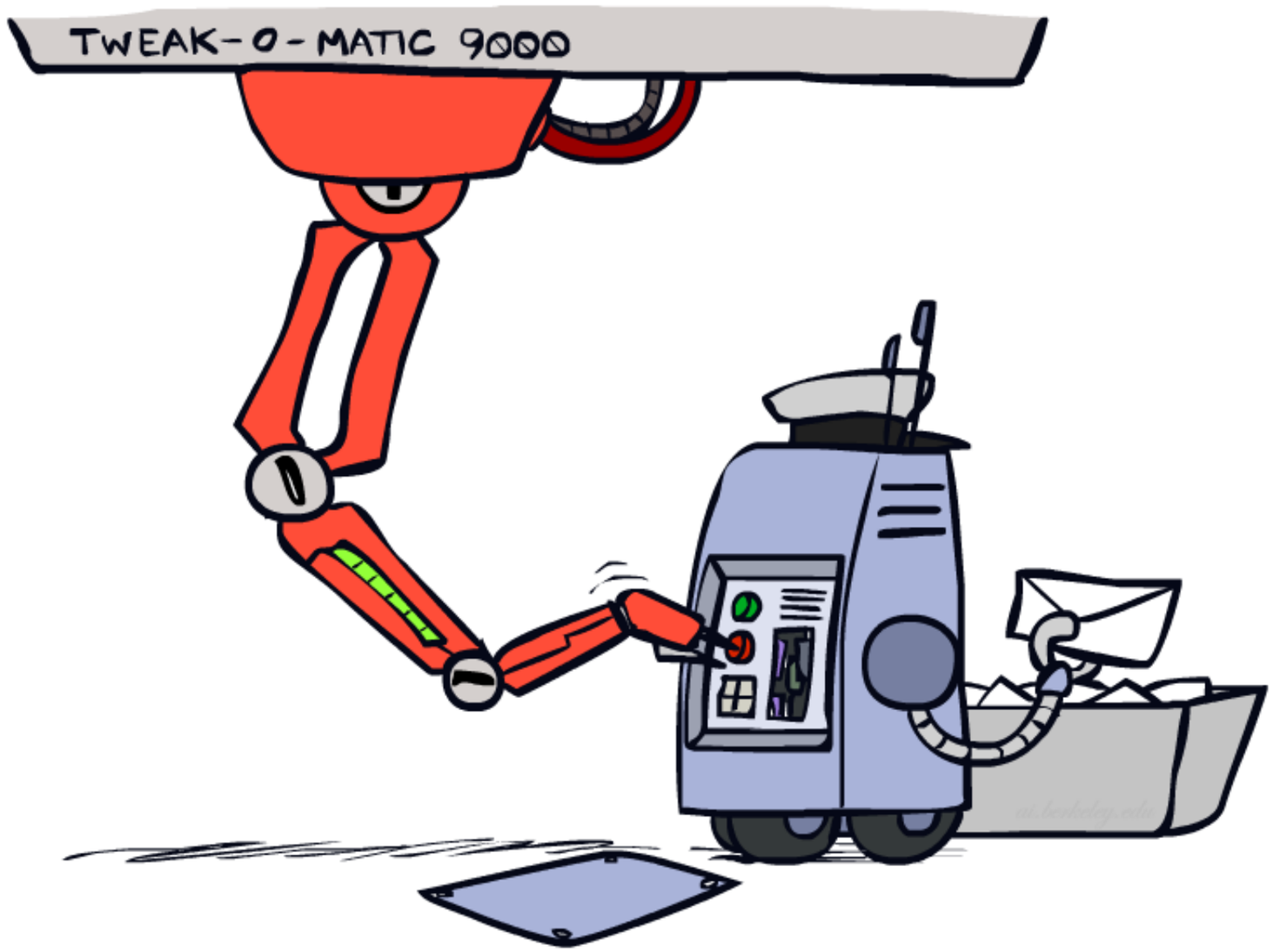
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

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



Do these make more sense?

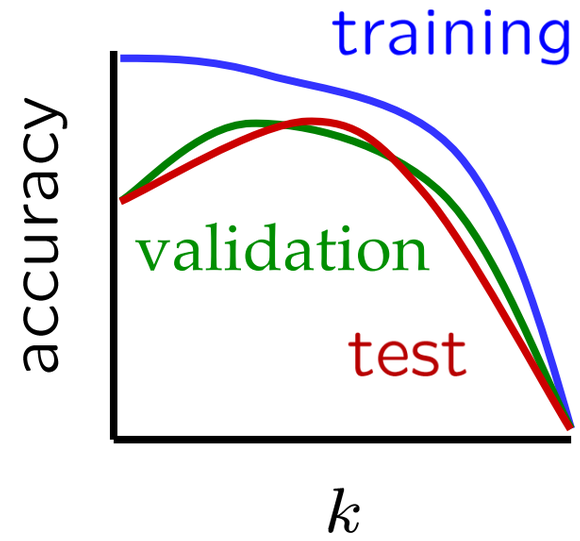
Tuning

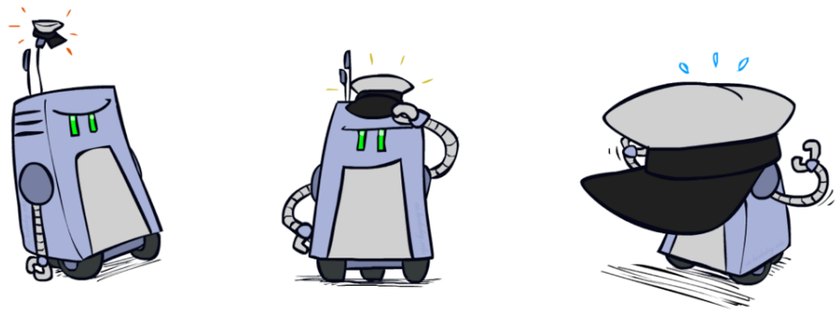


Tuning on Validation Data

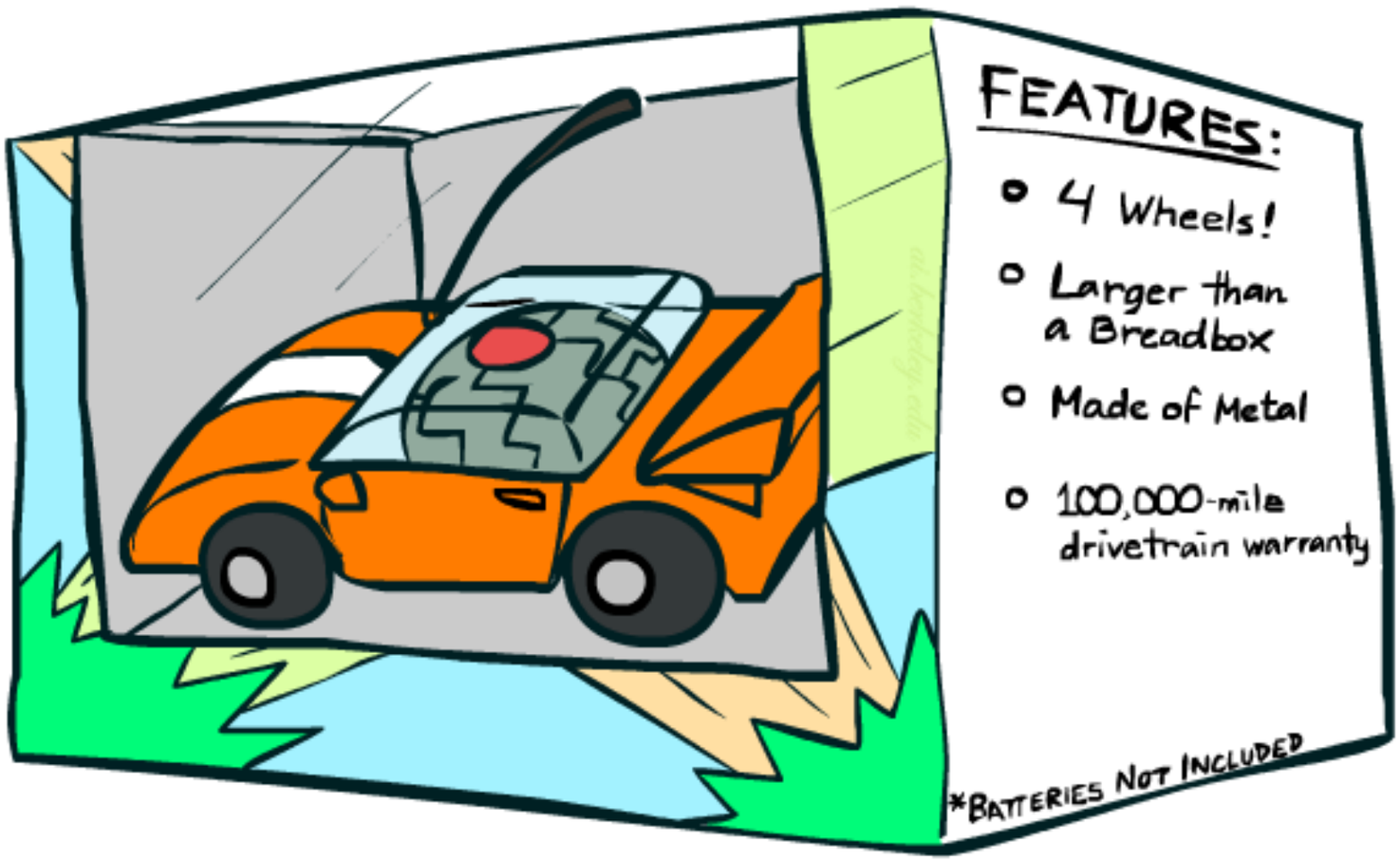
- Now we've got two kinds of unknowns
  - Parameters: the probabilities $P(X \mid Y)$, $P(Y)$
  - Hyperparameters: e.g., the amount / type of smoothing to do, k, α

- 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 validation 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 . . .
```

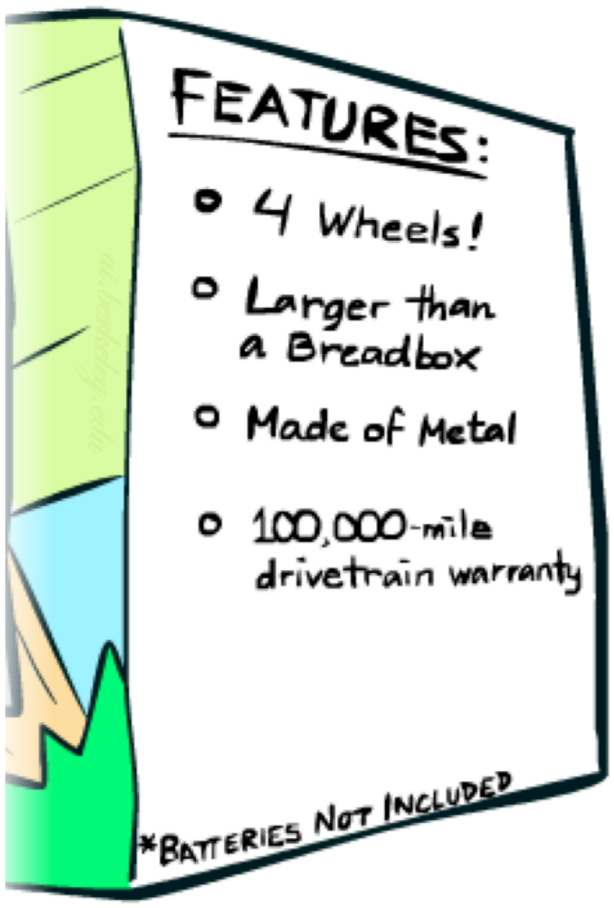
```
. . . To receive your $30 Amazon.com promotional
certificate, click through to

  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

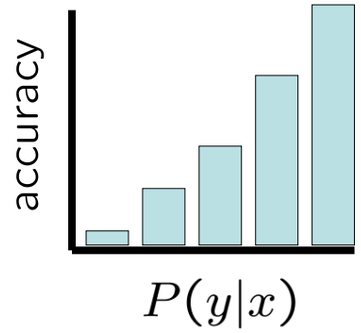
- Weak baseline: most frequent label classifier
  - Gives all test instances whatever label was most common in the training set
  - E.g. for spam filtering, might label everything as ham
  - Accuracy might be very high if the problem is skewed
  - E.g. calling everything "ham" gets 66%, so a classifier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

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

Confidences from a Classifier

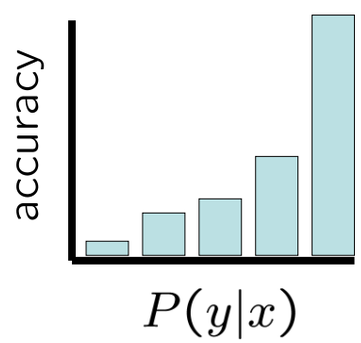
- The confidence of a probabilistic classifier:
  - Posterior over the top label

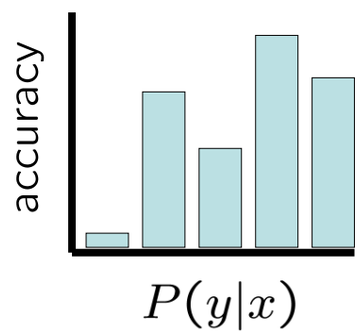
$$\text{confidence}(x) = \max_y P(y|x)$$



  - 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