

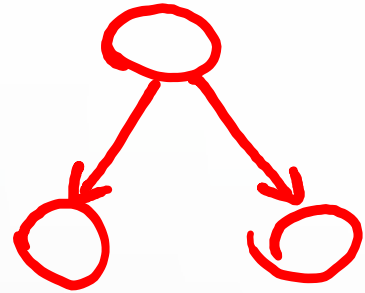


# Artificial Intelligence CE-417, Group 1 Computer Eng. Department Sharif University of Technology

Spring 2024

By Mohammad Hossein Rohban, Ph.D.

Courtesy: Most slides are adopted from CSE-573 (Washington U.), original slides for the textbook, and CS-188 (UC. Berkeley).



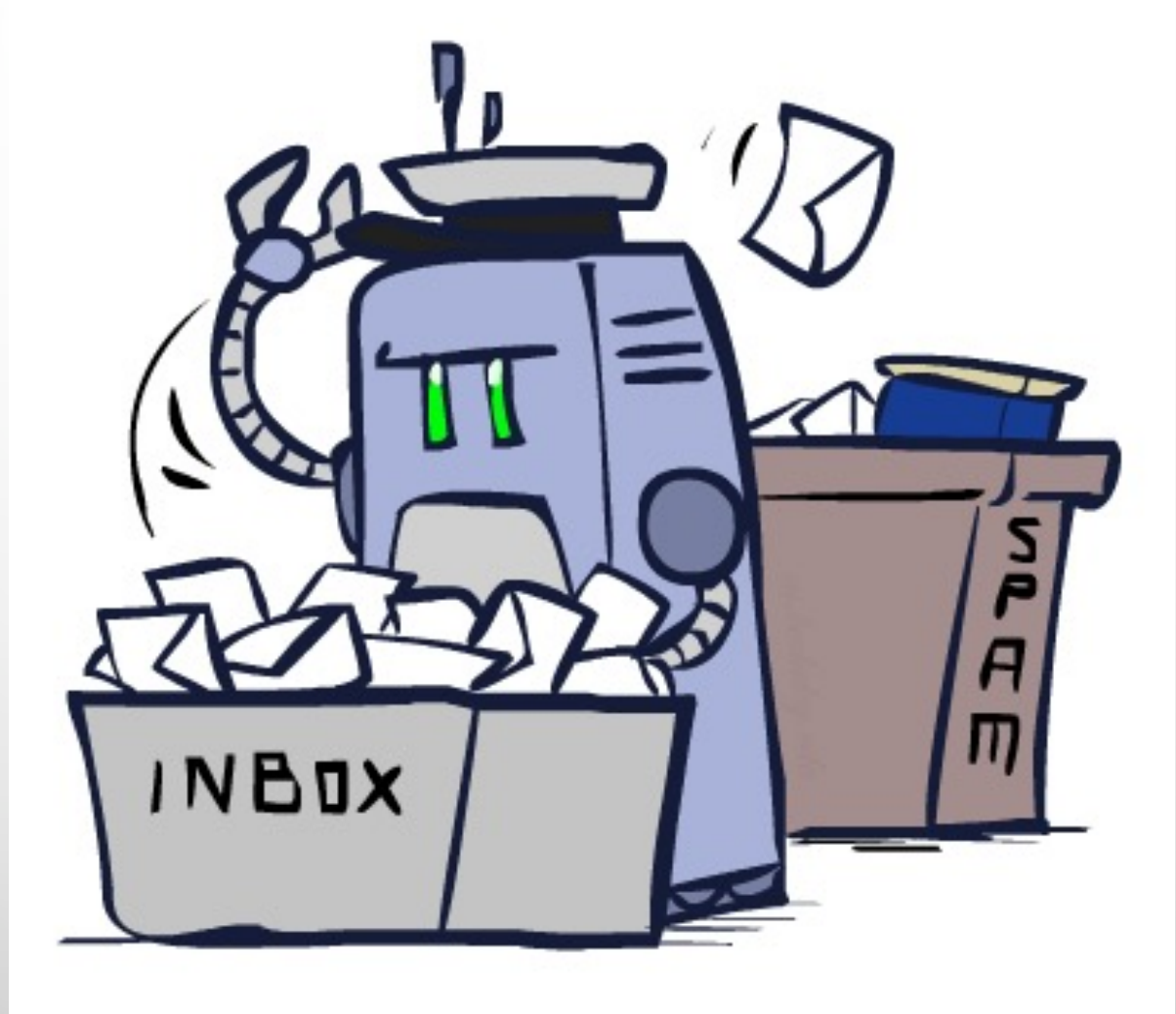
Machine Learning → Data

Key Concepts

*Generalization*

# Machine Learning

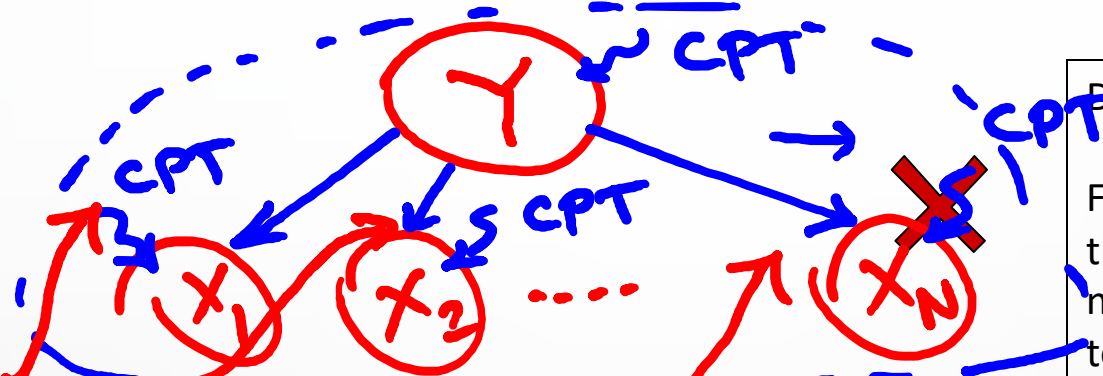
- Up until now: how use a model to make optimal decisions.
- Machine learning: how to acquire a model from data / experience
  - Learning parameters (e.g. Probabilities)
  - Learning structure (e.g. BN graphs)
  - Learning hidden concepts (e.g. Clustering)
- Today: model-based classification with naive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



$$P(Y | X_1, \dots, X_N)$$

# 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 virtue of its nature as being utterly confidential 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, I know 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.

**AI** Training Data → Estimation



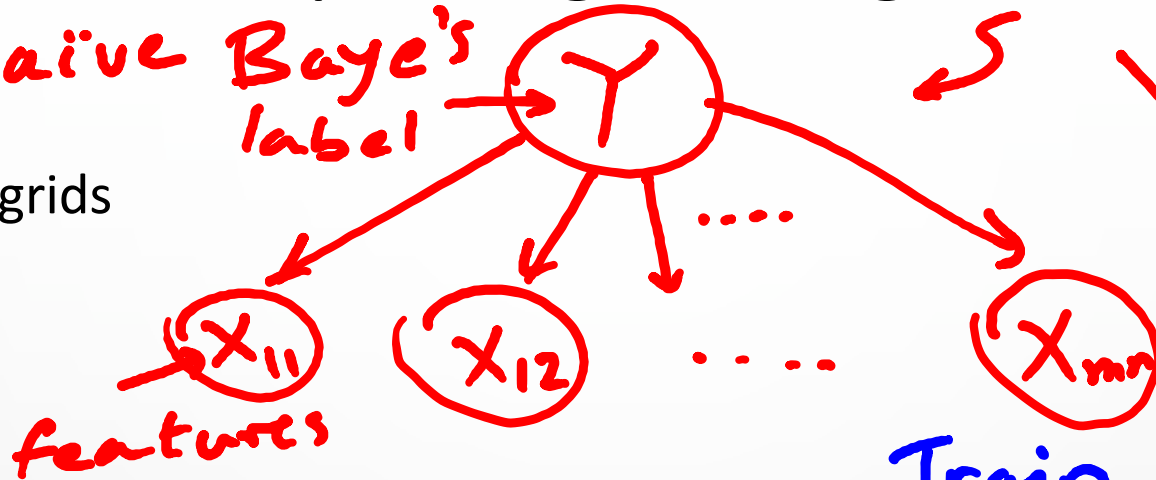
feature

# Example: Digit Recognition

Classification

Naive Baye's label

- 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

Clustering / Topic Modeling / LLM Test

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

feature	label
	0
	1
	2
	1
	??

Unsupervised L. vs. Reinforcement L.

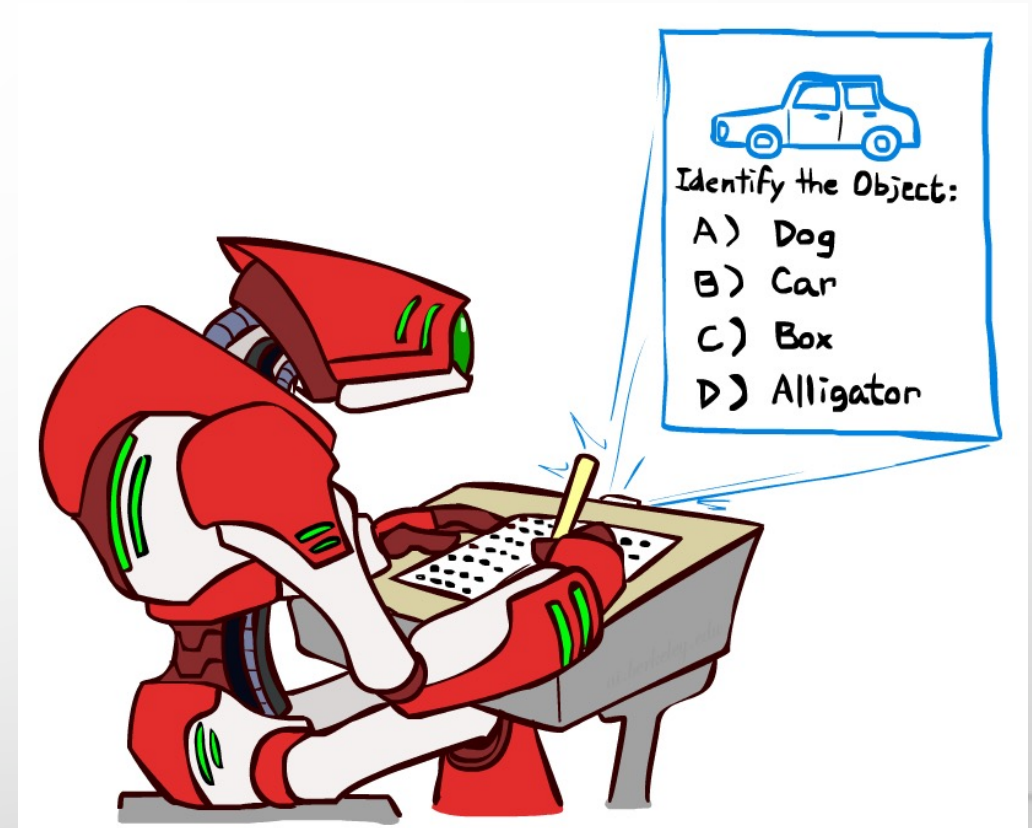
Supervised Learning

# 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!



feature

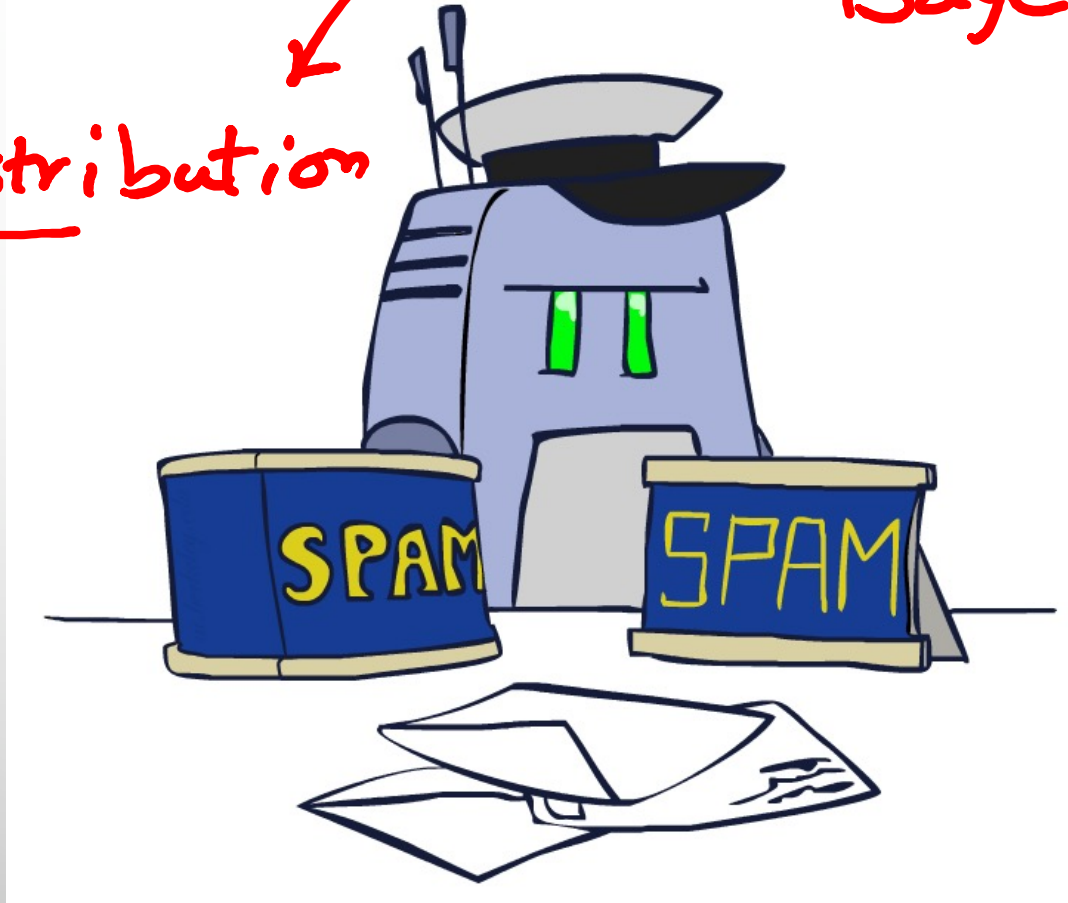
label

# Model-Based Classification

$X_1, \dots, X_d$     $Y$

Model: joint distribution

Baye's Net





# 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  $\langle i,j \rangle$
- 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.

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

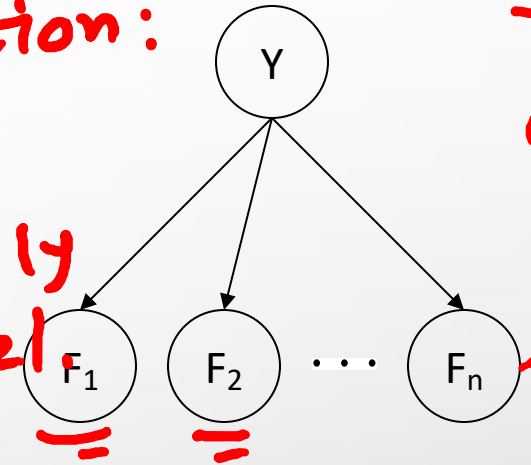
- Here: lots of features, each is binary valued

- Naïve Bayes model:

$$P(Y | F_{0,0} \dots F_{15,15}) \propto P(Y) \prod_{i,j} P(F_{i,j} | Y)$$

- What do we need to learn?

Assumption:  
features are dependent only through the label



$$P(F_{0,0} \dots F_{15,15} | Y) \rightarrow F_1 \perp\!\!\!\perp F_2 | Y$$

$$\begin{matrix} = 1 & = 1 \\ \vdots & \vdots \\ = 9 & = 9 \end{matrix} \left. \vphantom{\begin{matrix} = 1 \\ \vdots \\ = 9 \end{matrix}} \right\} 10$$

# General Naïve Bayes

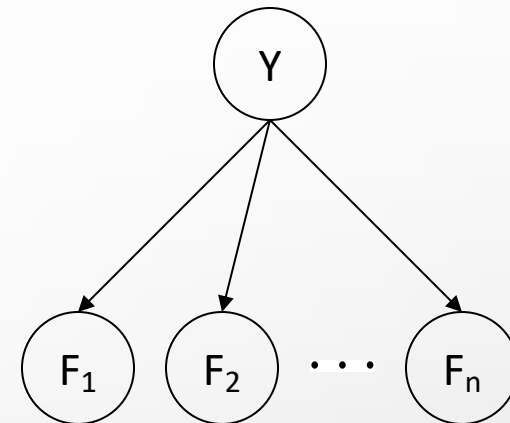
- A general **naive Bayes** model:

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

|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

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

---

$$P(f_1 \dots f_n)$$

+

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

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

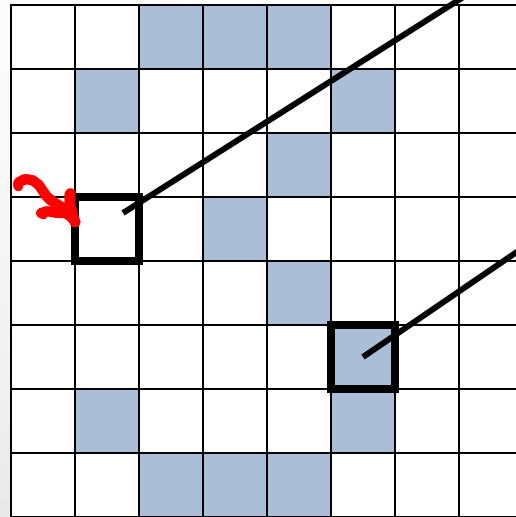
# General Naïve Bayes

- 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  $P(Y | F_1 \dots F_n)$
    - 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  $\theta$
    - Up until now, we assumed these appeared by magic, but...
    - ...They typically come from training data counts: we'll look at this soon

# Example: Conditional Probabilities

$P(Y)$

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



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

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

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

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

# Naïve Bayes for Text

- Bag-of-words naïve Bayes:

- Features:  $W_i$  is the word at position  $i$
- As before: predict label conditioned on feature variables (spam vs. Ham)
- As before: assume features are conditionally independent given label
- **New: each  $W_i$  is identically distributed**

- Generative model:

$$P(Y, W_1 \dots W_n) = P(Y) \prod_i P(W_i | Y)$$

*Word at position  $i$ , not  $i^{\text{th}}$  word in the dictionary!*

- “Tied” distributions and bag-of-words

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

# Example: Spam Filtering

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

$P(Y)$

ham	: 0.66
spam	: 0.33

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

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

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

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

- Where do these tables come from?

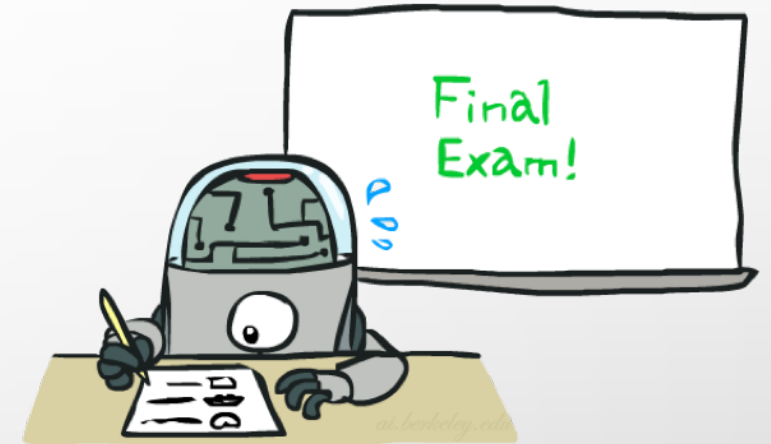
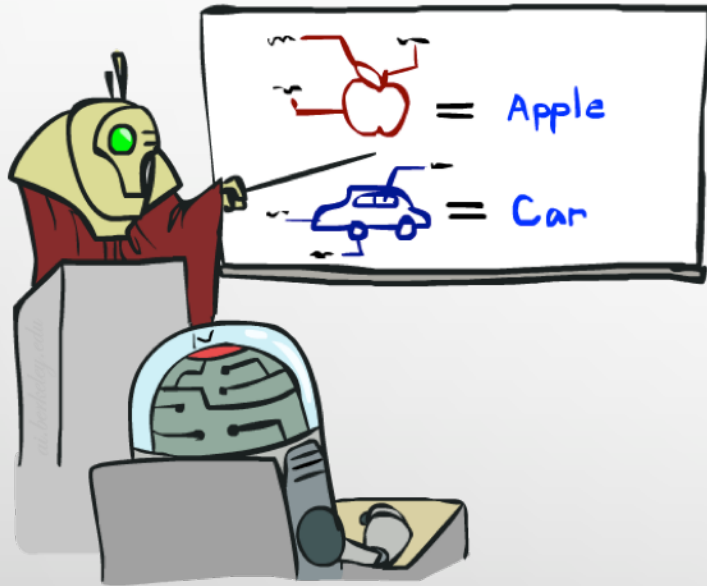


# Spam Example

Word	$P(w \text{spam})$	$P(w \text{ham})$	Tot Spam	Tot Ham
(prior)	0.33333	0.66666	-1.1	-0.4

$$P(\text{spam} | w) = 98.9$$

# Training and Testing



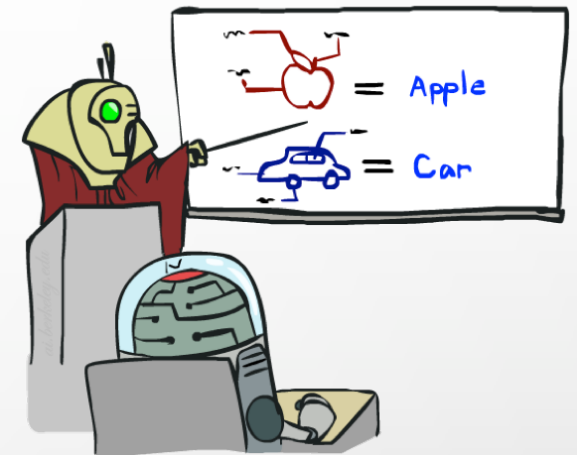
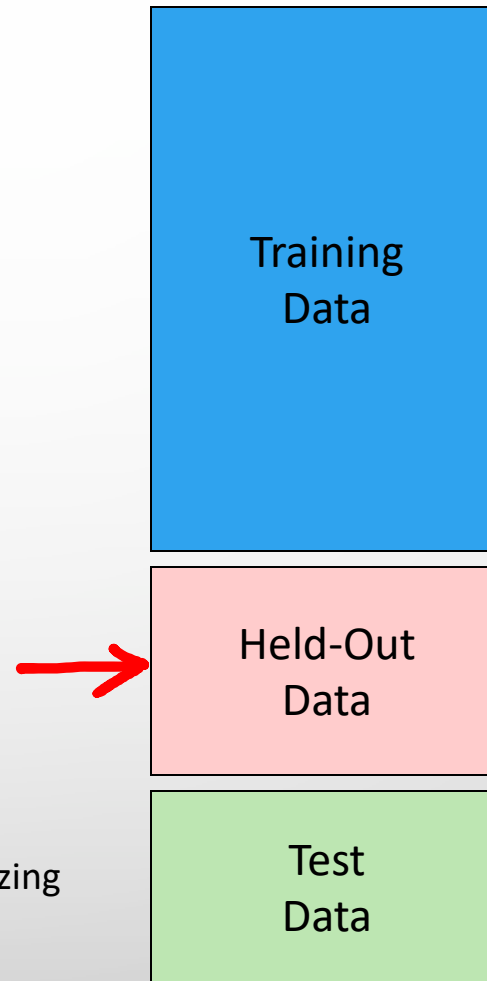
# Hyperparameter vs. Parameter

## Important Concepts

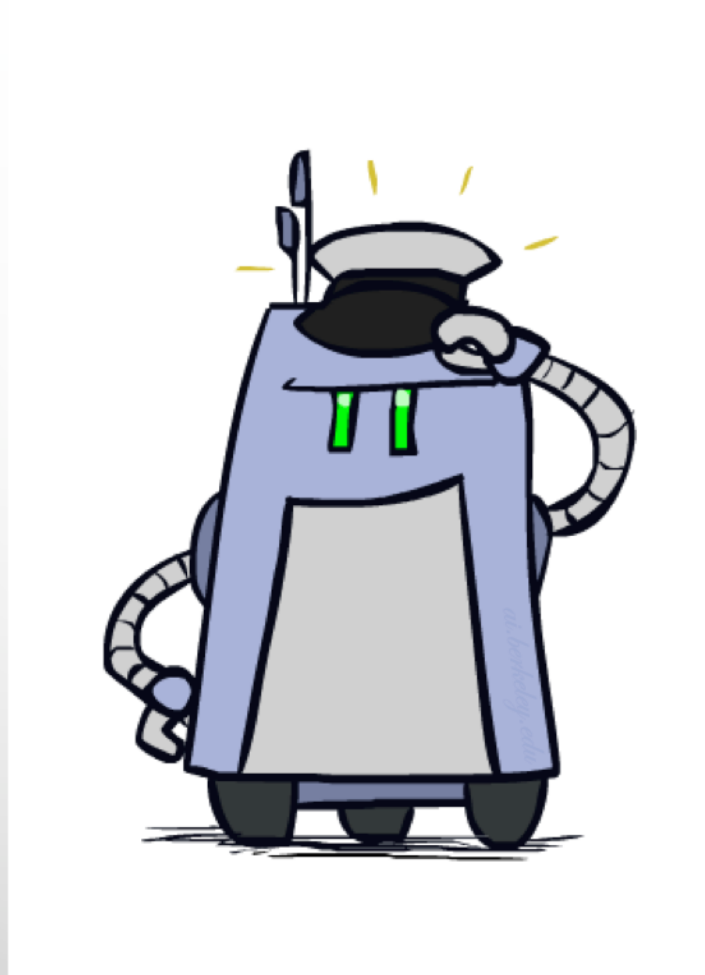
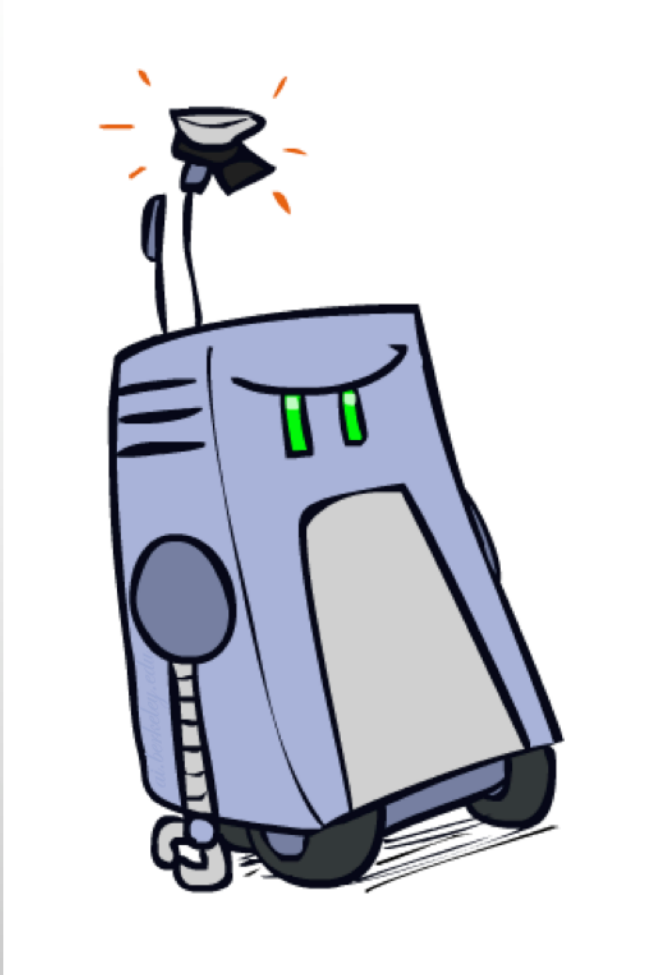
← K → Laplace Smoothing

- 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

Validation Set



# Generalization and Overfitting



# Overfitting

30

25

20

Degree 15 polynomial

15

10

5

0

-5

-10

-15

0

2

4

6

8

10

12

14

16

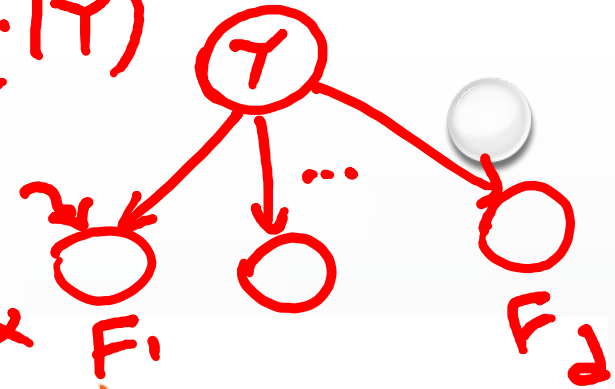
18

20



# Example: Overfitting

$$P(\underline{x}_i | Y)$$



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

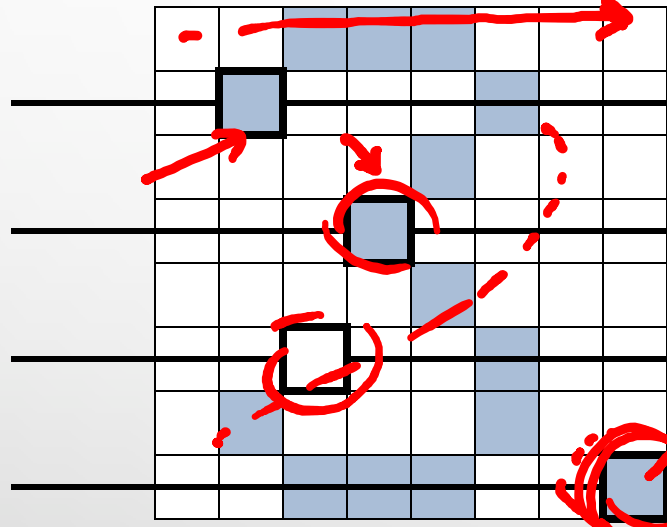
$P(C = 2) = 0.1$

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

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

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

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



2 wins!!

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

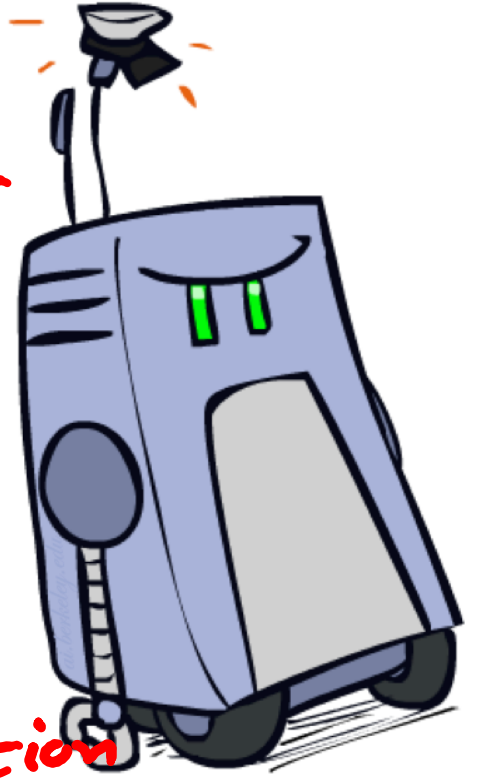
$P(C = 3) = 0.1$

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

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

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

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



point estimation vs. interval estimation

# Example: Overfitting

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

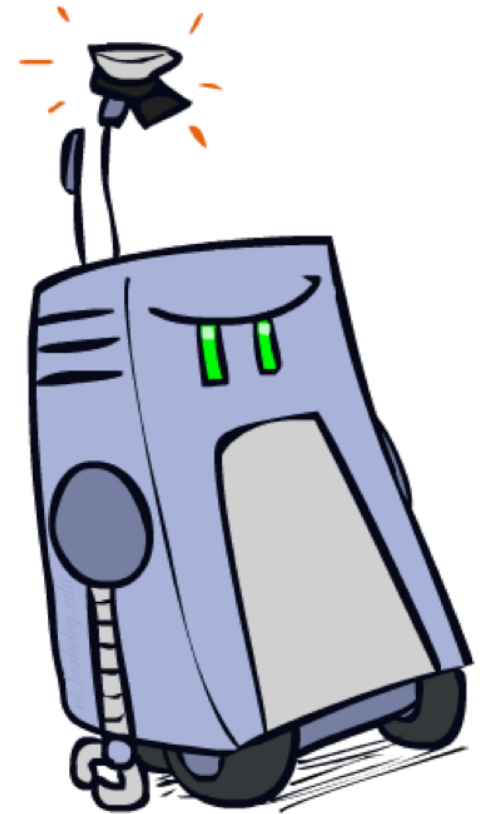
$$\frac{P(W|\text{ham})}{P(W|\text{spam})}$$

```
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?*

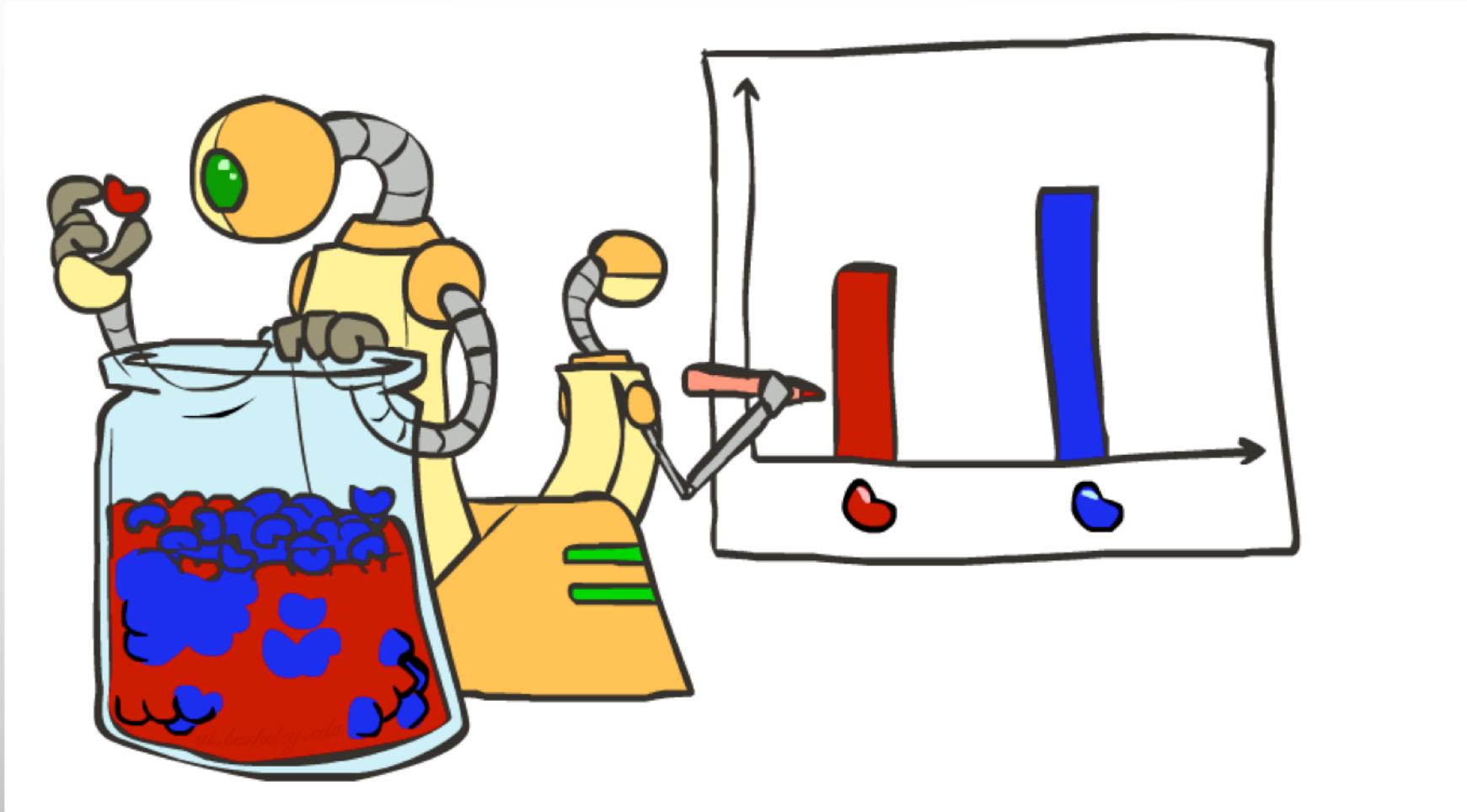


# Generalization and Overfitting

- 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



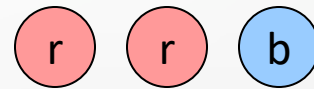
# Parameter Estimation



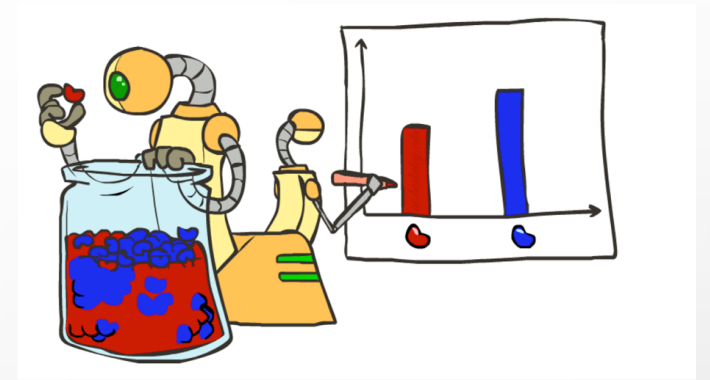
# Parameter Estimation

- 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:

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



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



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

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

# Maximum Likelihood

$$P_{\theta}(x) = \theta^x (1-\theta)^{1-x} \quad x \in \{0, 1\}$$

Likelihood

$\rightarrow X_1 \dots X_n \stackrel{iid}{\sim} P_{\theta}(x)$

$$\max_{\theta} P(X_1, \dots, X_n | \theta)$$

$$\max_{\theta} \prod_{i=1}^n \theta^{x_i} (1-\theta)^{1-x_i}$$

$$\equiv \max_{\theta} \sum x_i \log \theta$$

$$\prod_{i=1}^n P(x_i | \theta) + (1-x_i) \log(1-\theta)$$

$$\sum \frac{x_i}{\theta} + (1-x_i) \left( \frac{-1}{1-\theta} \right) = 0$$

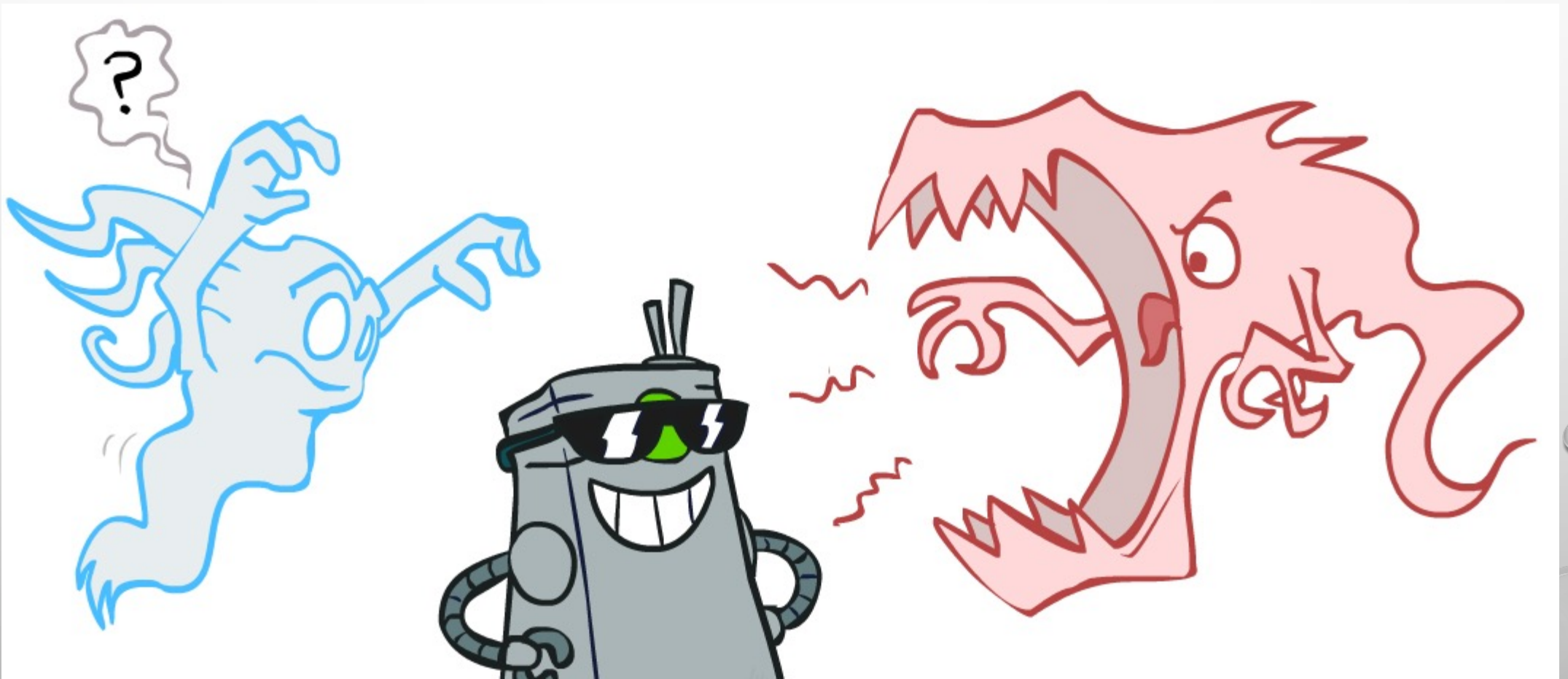
$$\rightarrow \theta = \frac{1}{n} \sum_{i=1}^n x_i$$

Dirichlet

$\rightarrow P(\theta) \rightsquigarrow$  prior prob.

$$P(\theta | X_1, \dots, X_n) \propto P(X_1, \dots, X_n | \theta) P(\theta)$$

# Smoothing



# Maximum Likelihood?

- Relative frequencies are the maximum likelihood estimates

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

$$= \arg \max_{\theta} \prod_i P_{\theta}(X_i)$$

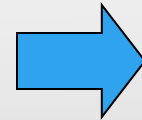


$$P_{ML}(x) = \frac{\text{count}(x)}{\text{total samples}}$$

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

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

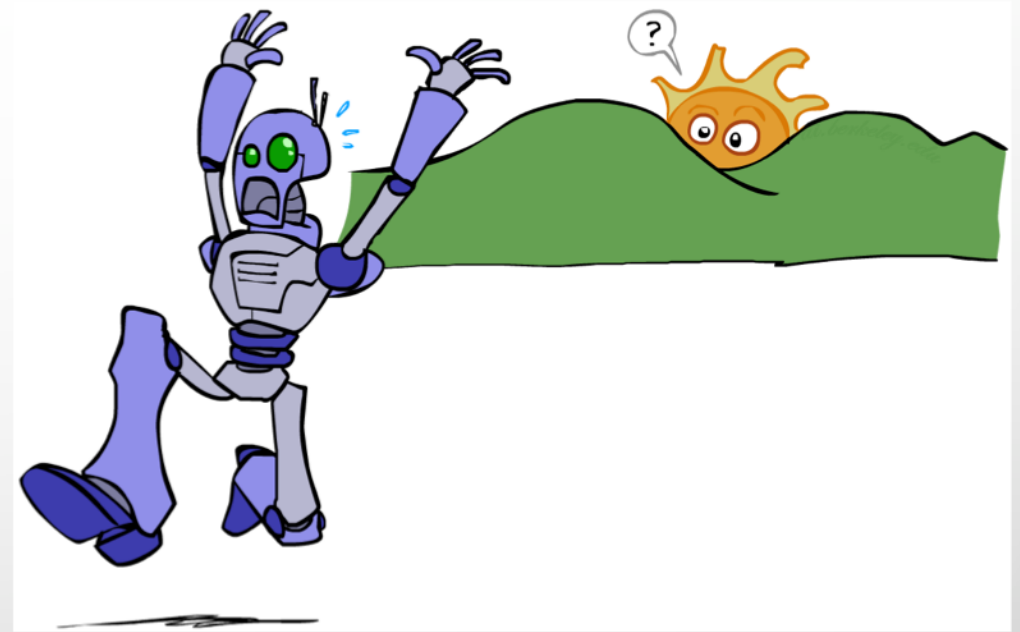
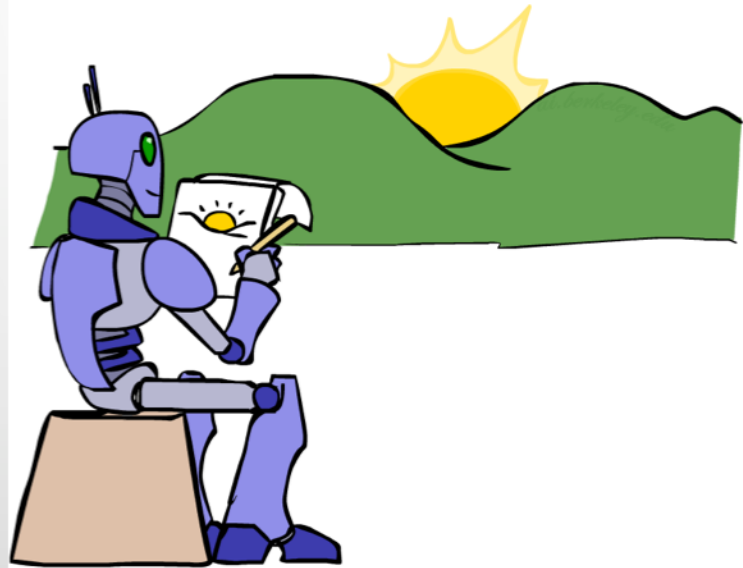
$$= \arg \max_{\theta} P(\mathbf{X}|\theta)P(\theta)/P(\mathbf{X})$$



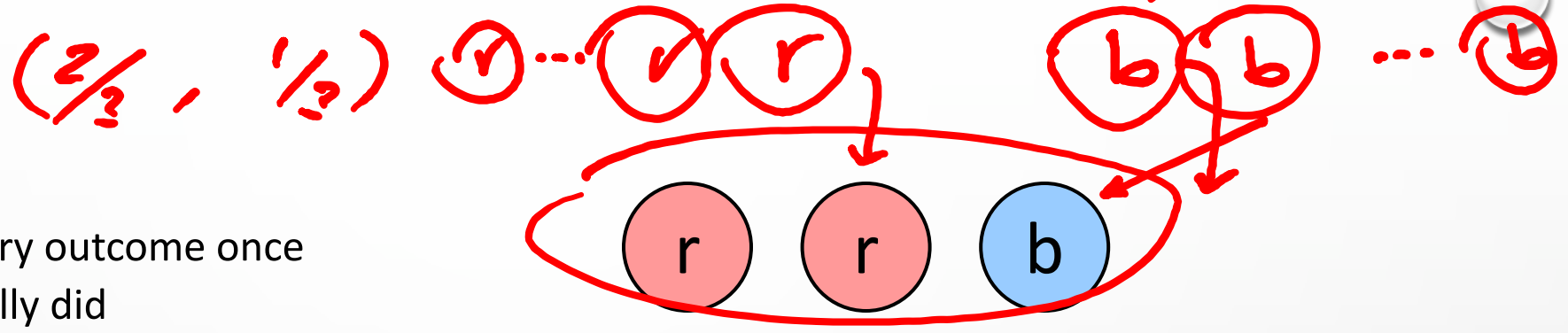
????

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

# 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 *Probabilistic Graphical Models course*)

# Laplace Smoothing

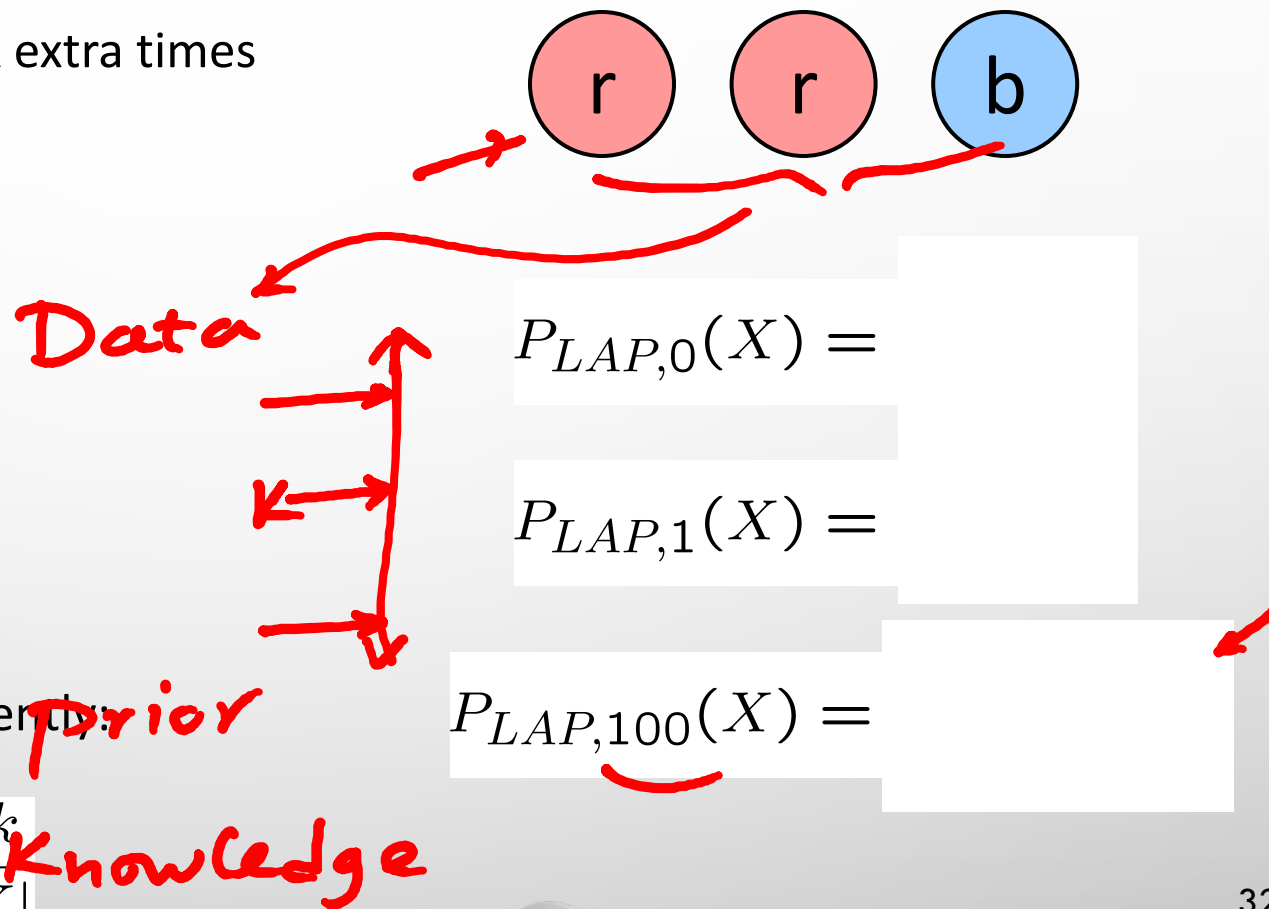
- Laplace's estimate (extended):
  - Pretend you saw every outcome  $k$  extra times

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

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

- Laplace for conditionals:
  - Smooth each condition independently:

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





# Estimation: Linear Interpolation

- In practice, Laplace often performs poorly for  $P(X_i|Y)$ :

- When  $|X|$  is very large
- When  $|Y|$  is very large

- Another option: linear interpolation

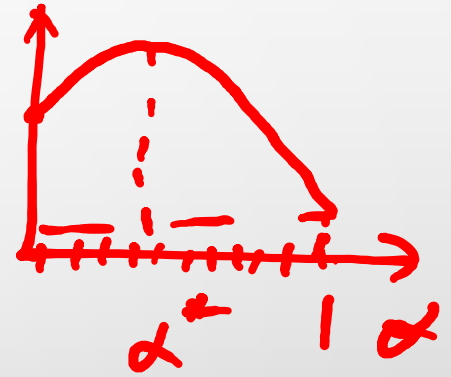
- Also get the empirical  $P(X)$  from the data
- Make sure the estimate of  $P(X|Y)$  isn't too different from the empirical  $P(X)$

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

- What if  $\alpha$  is 0? 1?
- See *Stochastic Processes* course for more interesting options of making the estimation.

$$0 \leq \alpha \leq 1$$

Held out Acc



# 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
...		

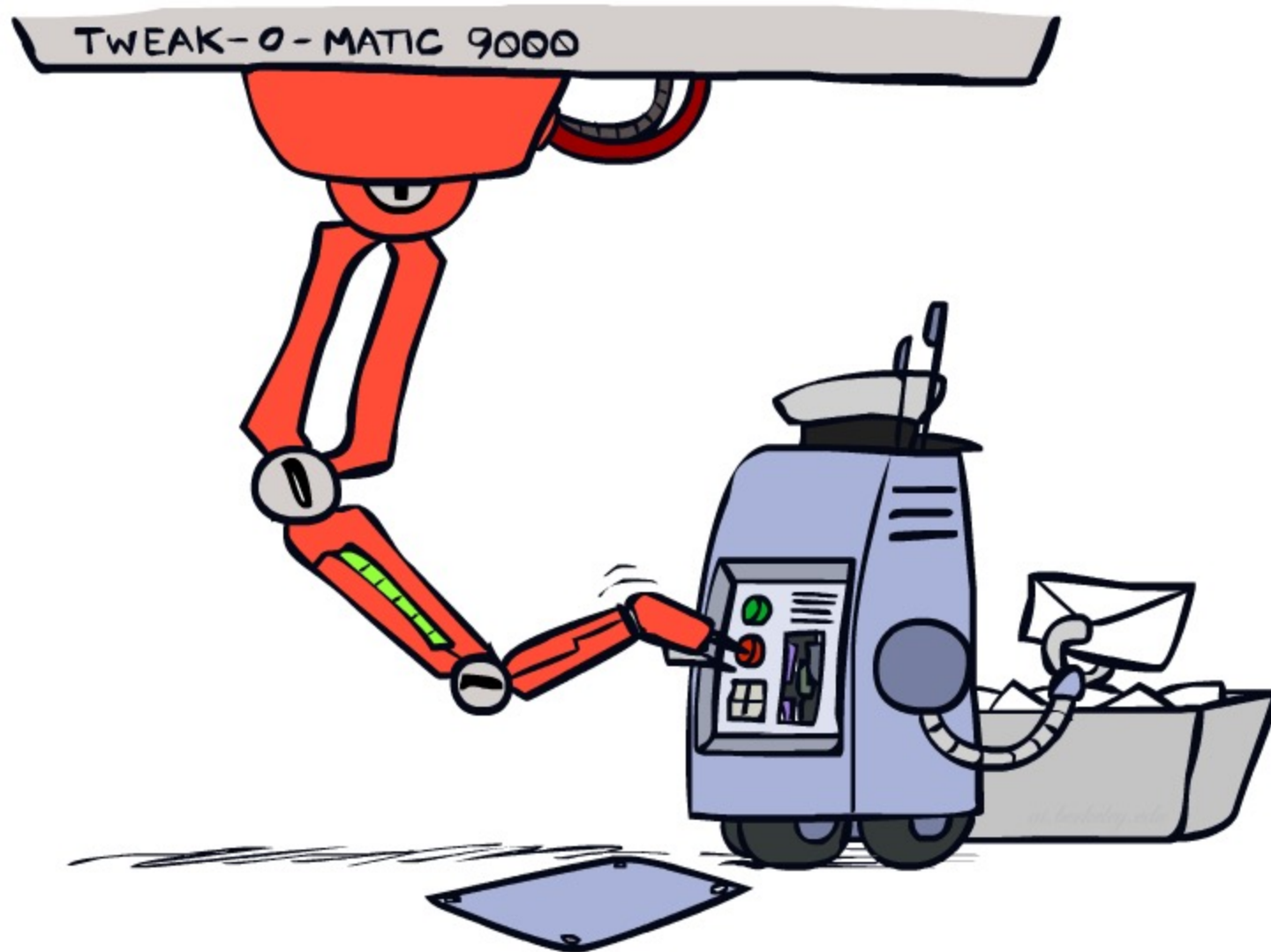
$$\frac{P(W|\text{spam})}{P(W|\text{ham})}$$

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

*Do these make more sense?*



# Tuning



naive Bayes

# Tuning on Held-Out Data

Decision Tree

- 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,  $k$ ,  $\alpha$
- 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

