Artificial Intelligence
CE-417, Group 2
Computer Eng. Department
Sharif University of Technology

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

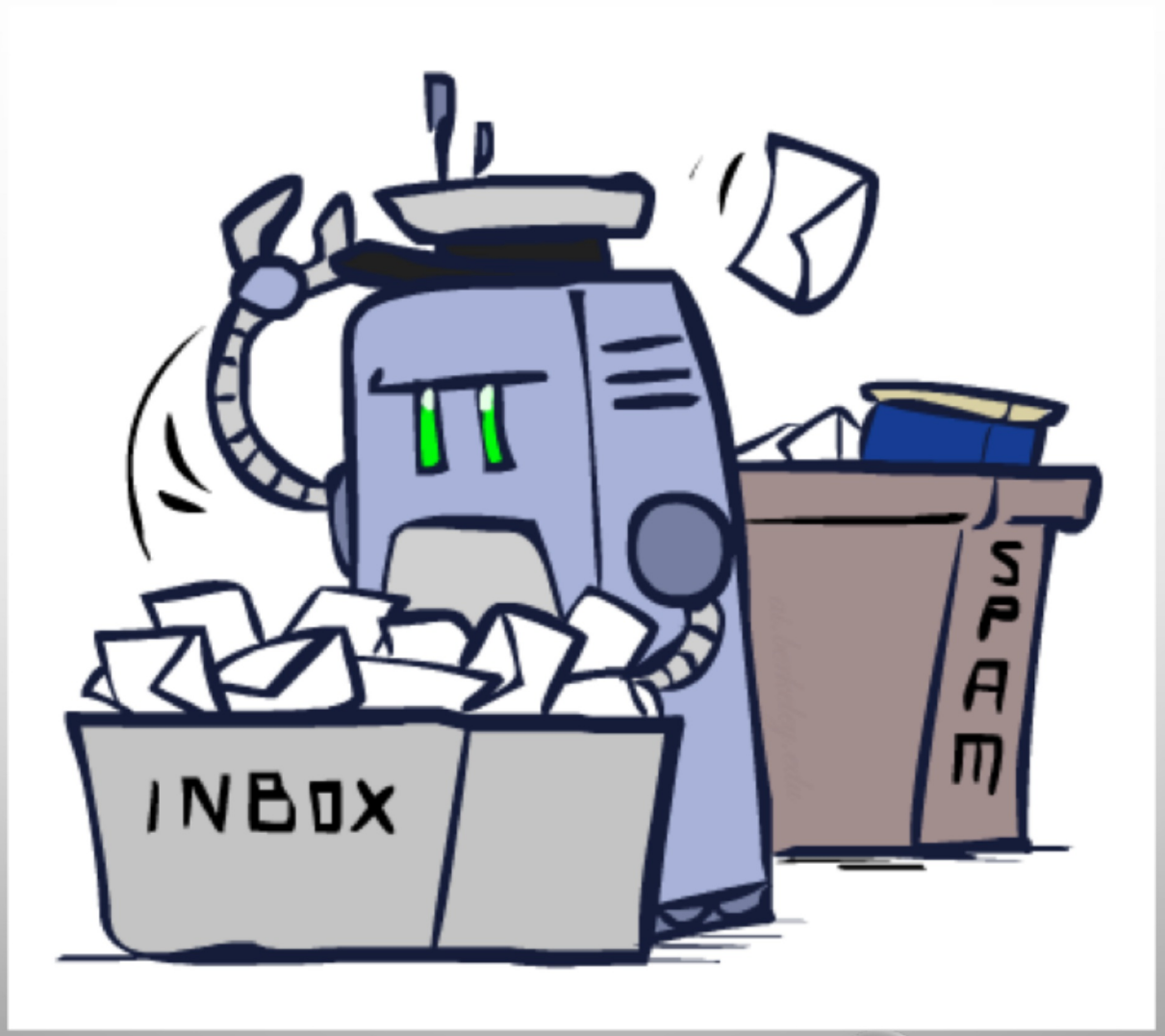
Machine Learning

Key Concepts

Machine Learning

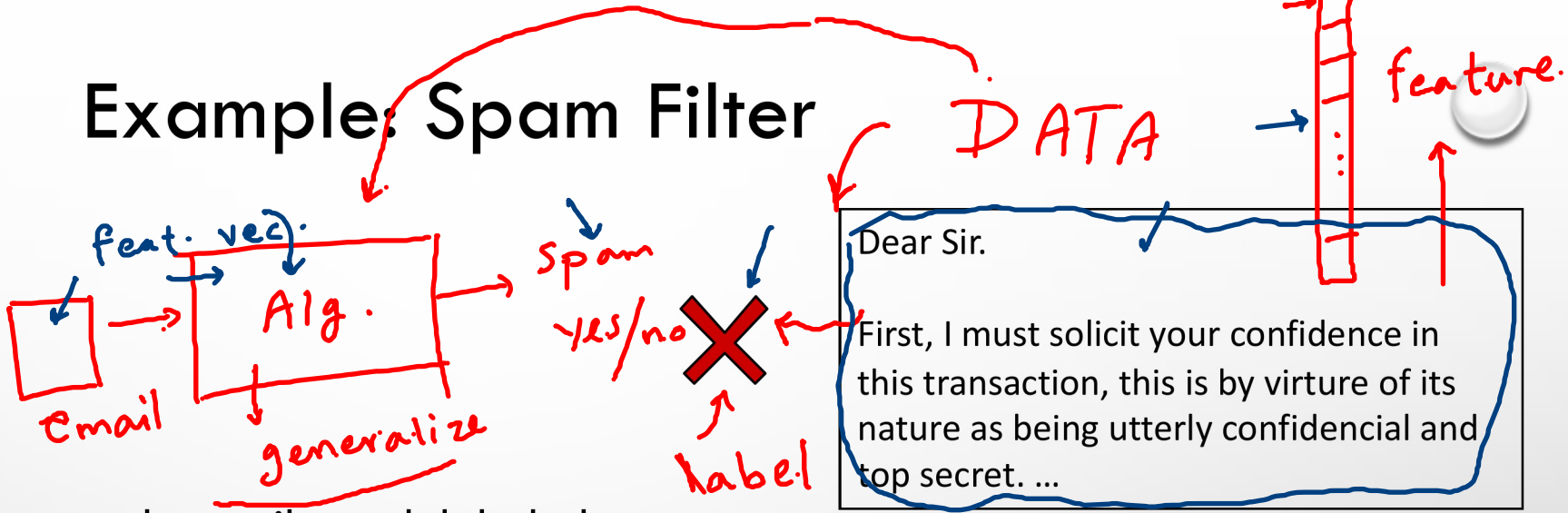
- Up until now: how use a model to make optimal decisions.
- Machine learning: how to acquire a model from data / experience
  - Learning parameters (e.g. Probabilities)
  - Learning structure (e.g. BN graphs)
  - Learning hidden concepts (e.g. Clustering)

- Today: model-based classification with naive Bayes


INBOX
SPACE

Example: Spam Filter

- Input: an email
- Output: spam/ham

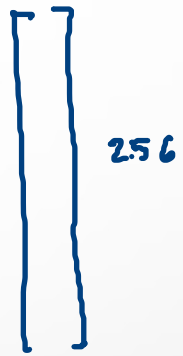


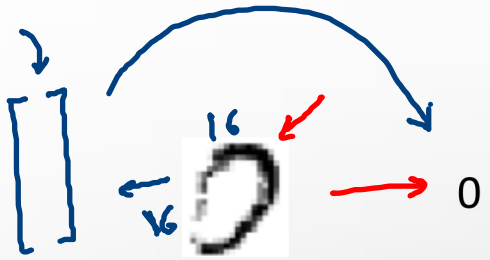
- Setup:
  - Get a large collection of example emails, each labeled "spam" or "ham"
  - Note: someone has to hand label all this data!
  - Want to learn to predict labels of new, future emails

- Features: the attributes used to make the ham / spam decision
  - Words: FREE!
  - Text patterns: $dd, CAPS
  - Non-text: SenderInContacts
  - …

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

develop prob. model on relevant variables → inference → predict the class

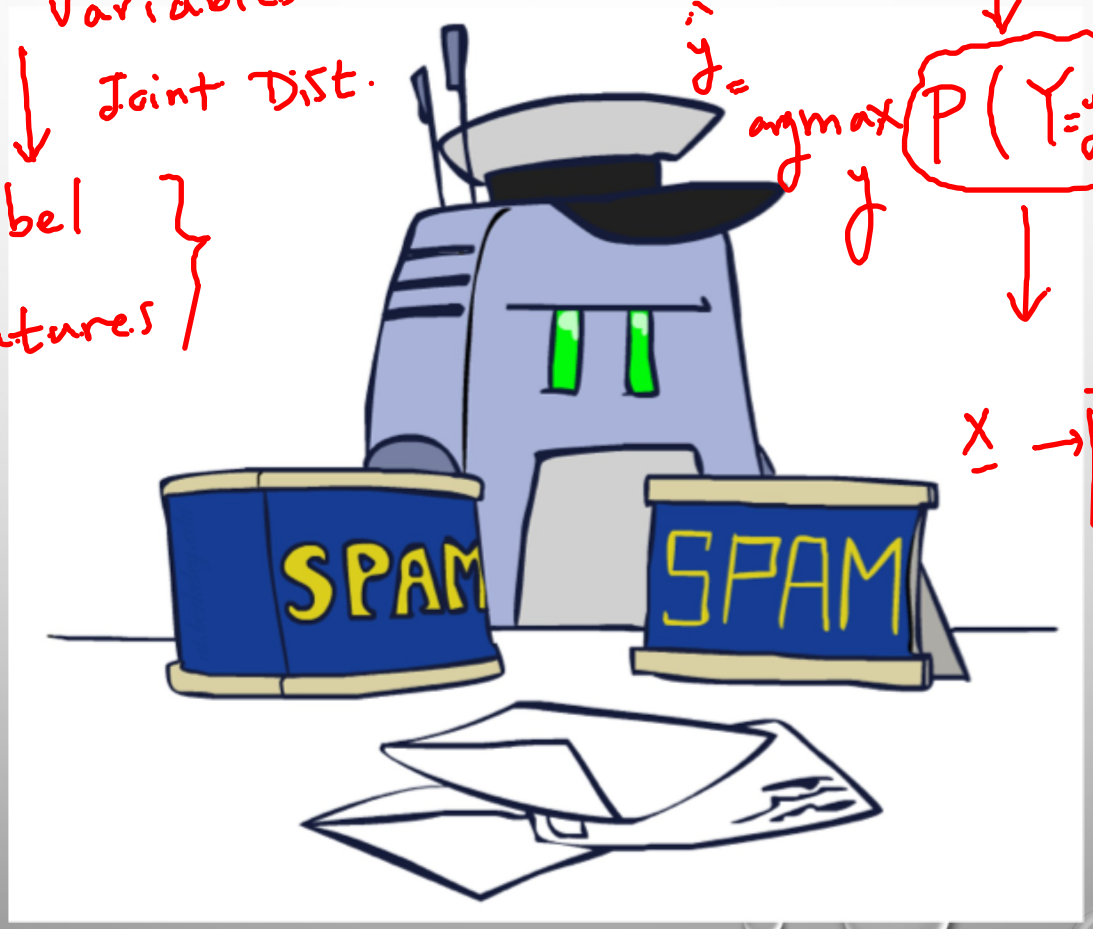
Joint Dist.

label } Y

features } $(X_1, \ldots, X_d) = \underline{X}$

$\hat{y} = \underset{y}{\operatorname{argmax}} P(Y=y \mid \underline{X}) = ?$

$\underline{X} \rightarrow$ Alg. $\rightarrow \hat{\underline{y}}$

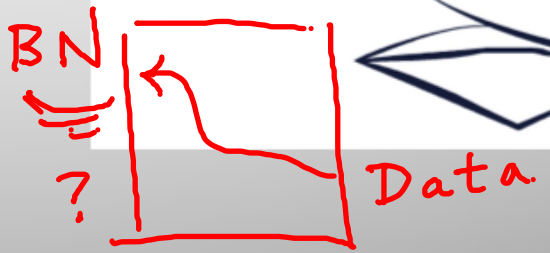


Model-Based Classification

- 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

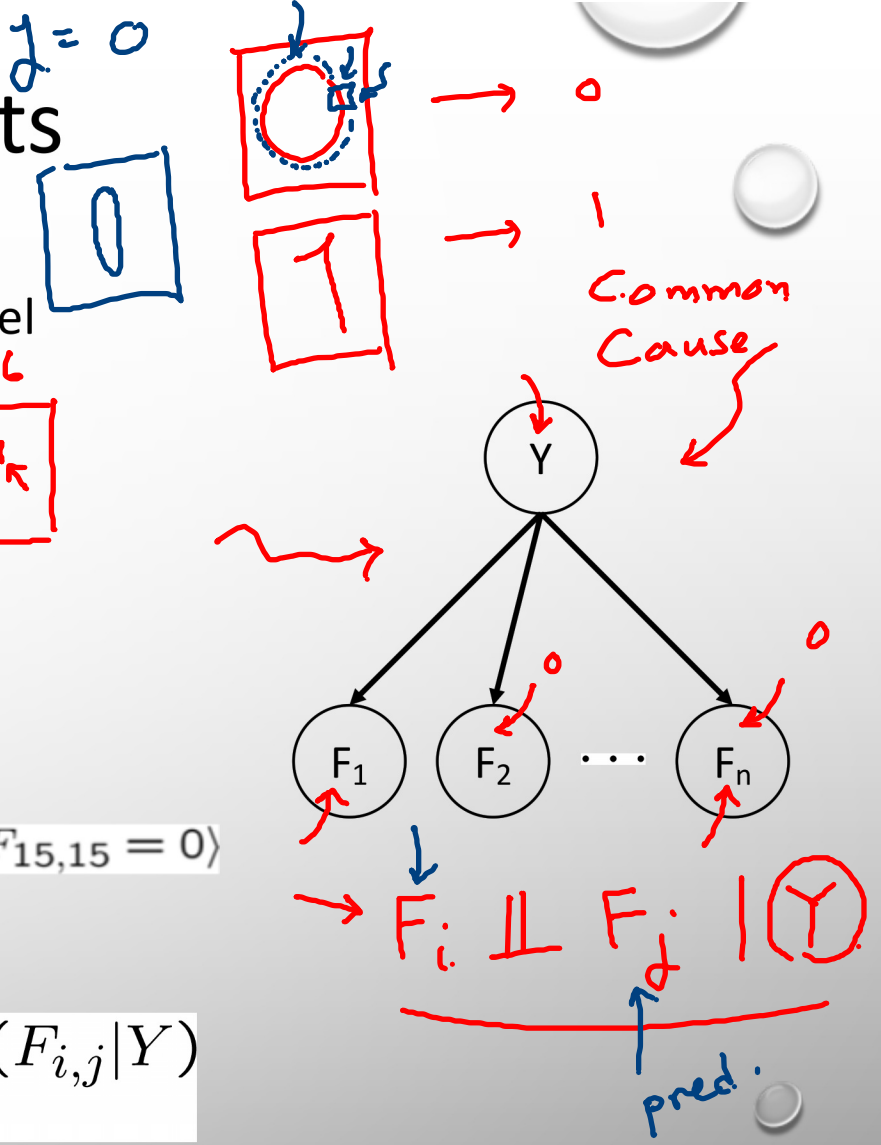
pred: $P(y \mid X)$ ← $P(X, y)$

- Challenges
  - What structure should the BN have?
  - How should we learn its parameters?



Learning

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:

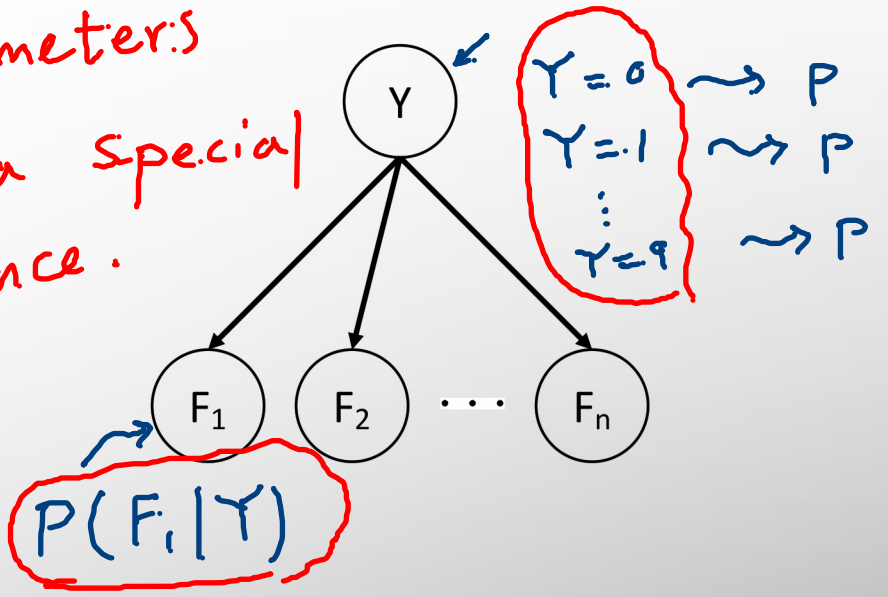
Reduction of free parameters is of a special importance.

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

|Y| parameters

|Y| x |F|^n values

n x |F| x |Y| parameters



→ generalization

- We only have to specify how each feature depends on the class
- Total number of parameters is *linear* in n → need ~ # of data points.
- 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

$$P(Y, f_1 \dots f_n) = \begin{bmatrix} P(y_1, f_1 \dots f_n) \\ P(y_2, f_1 \dots f_n) \\ \vdots \\ P(y_k, f_1 \dots f_n) \end{bmatrix} \xrightarrow{\text{BN}} \begin{bmatrix} P(y_1) \prod_i P(f_i|y_1) \\ P(y_2) \prod_i P(f_i|y_2) \\ \vdots \\ P(y_k) \prod_i P(f_i|y_k) \end{bmatrix} \Big/ P(f_1 \dots f_n)$$

$$\downarrow$$

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

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

$$\hat{y} = \operatorname{argmax}_y P(Y|f_1 \dots f_n)$$

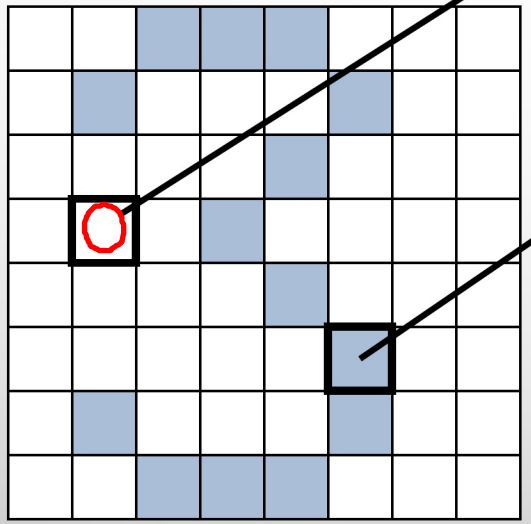
General Naïve Bayes

- What do we need in order to use naïve Bayes?
  - ✓ Inference method (we just saw this part)
    - Start with a bunch of probabilities: P(Y) and the $P(F_i|Y)$ tables
    - Use standard inference to compute $P(Y|F_1 \ldots F_n)$
    - Nothing new here
  - Estimates of local conditional probability tables (CPT ?)
    - P(Y), the prior over labels
    - $P(F_i|Y)$ for each feature (evidence variable)
    - These probabilities are collectively called the *parameters* of the model and denoted by θ
    - Up until now, we assumed these appeared by magic, but…
    - …They typically come from training data counts: we'll look at this soon

Example: Conditional Probabilities

$P(Y)$

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



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

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

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

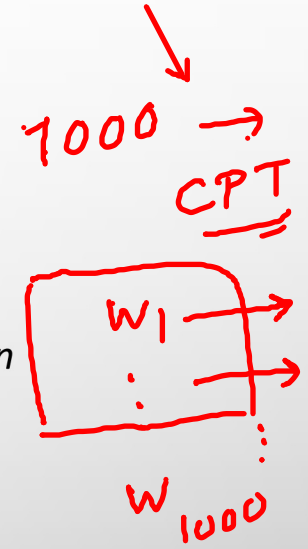
1	0.05
2	0.01
3	0.90
4	0.80
5	0.90
6	0.90
7	0.25
8	0.85
9	0.60
0	0.80

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 ith 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
...	

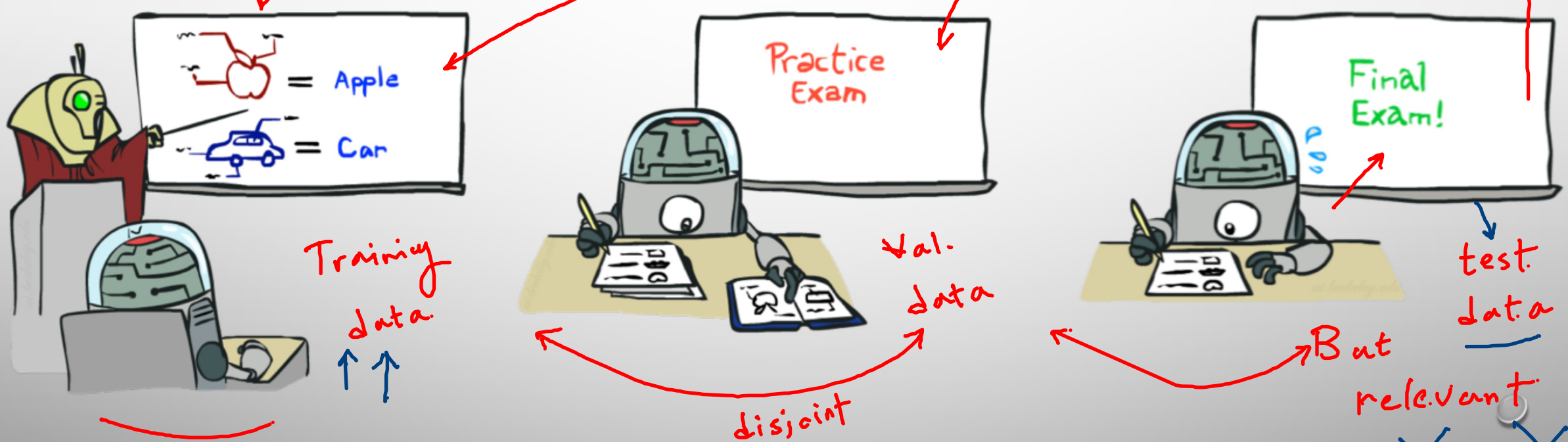
- Where do these tables come from?

Spam Example

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

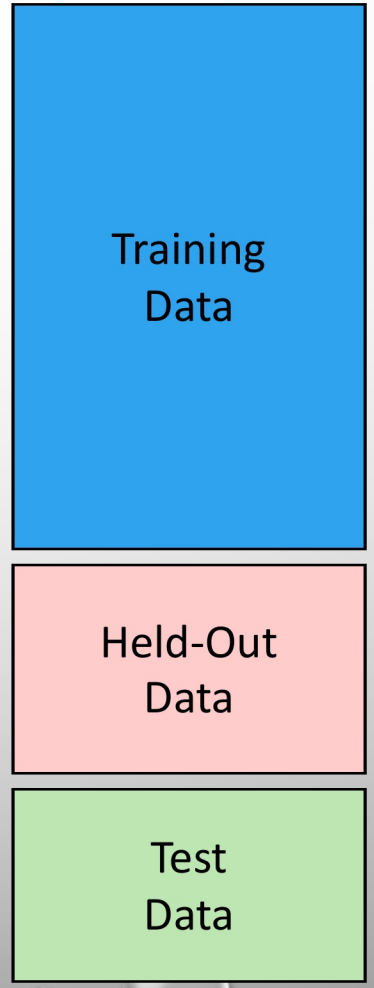
P(spam | w) = 98.9

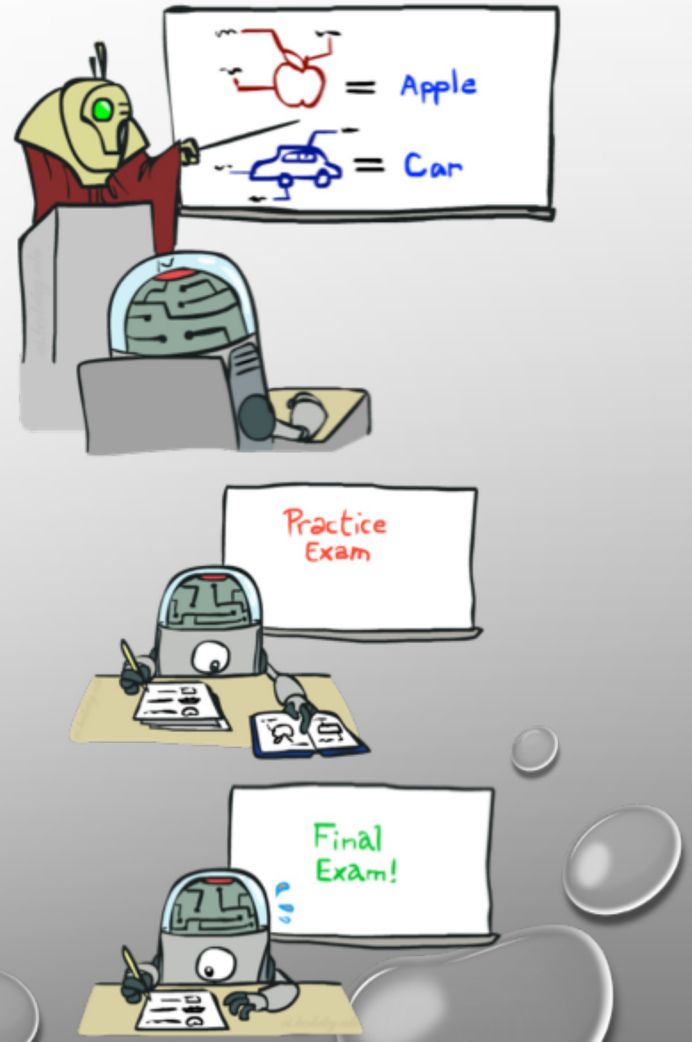
Training and Testing



Important Concepts

- Data: labeled instances, e.g. Emails marked spam/ham
  - Training set
  - Held out set
  - Test set
- Features: attribute-value pairs which characterize each x
- Experimentation cycle
  - Learn parameters (e.g. model probabilities) on training set
  - (Tune hyperparameters on held-out set)
  - Compute accuracy of test set
  - Very important: never "peek" at the test set!
- Evaluation
  - Accuracy: fraction of instances predicted correctly
- Overfitting and generalization
  - Want a classifier which does well on *test* data
  - Overfitting: fitting the training data very closely, but not generalizing well
  - We'll investigate overfitting and generalization formally in a few lectures

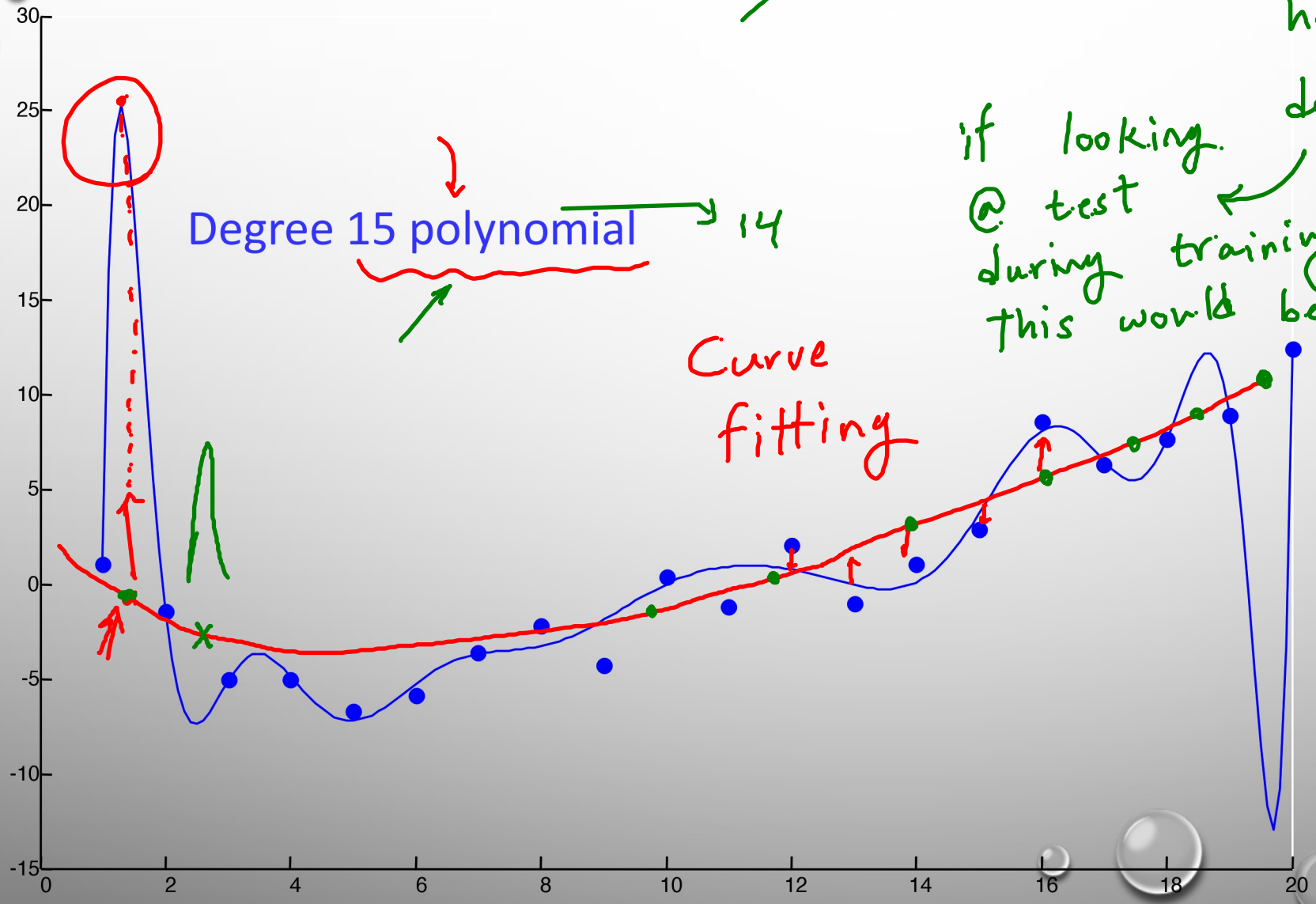




Generalization and Overfitting

Overfitting

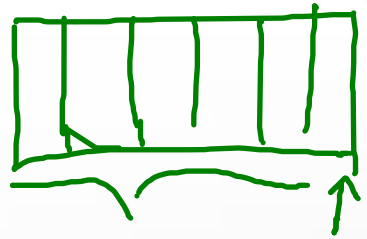
test set helps us to detect overfitting.

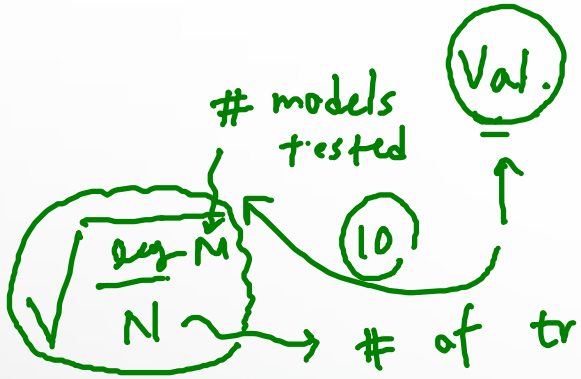


if looking @ test during training this would be destroyed!

K-fold Cross-Validation

Example: Overfitting





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

$P(C = 2) = 0.1$

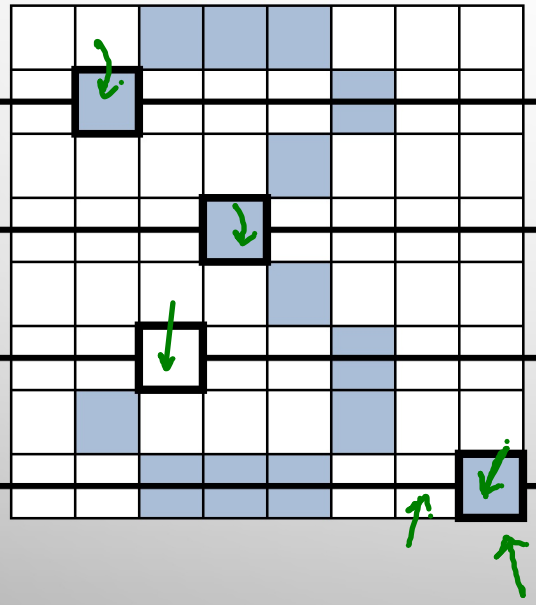
$P(\text{on}|C = 2) = 0.8$

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

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

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

> 0



2 wins!!

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

$P(C = 3) = 0.1$

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

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

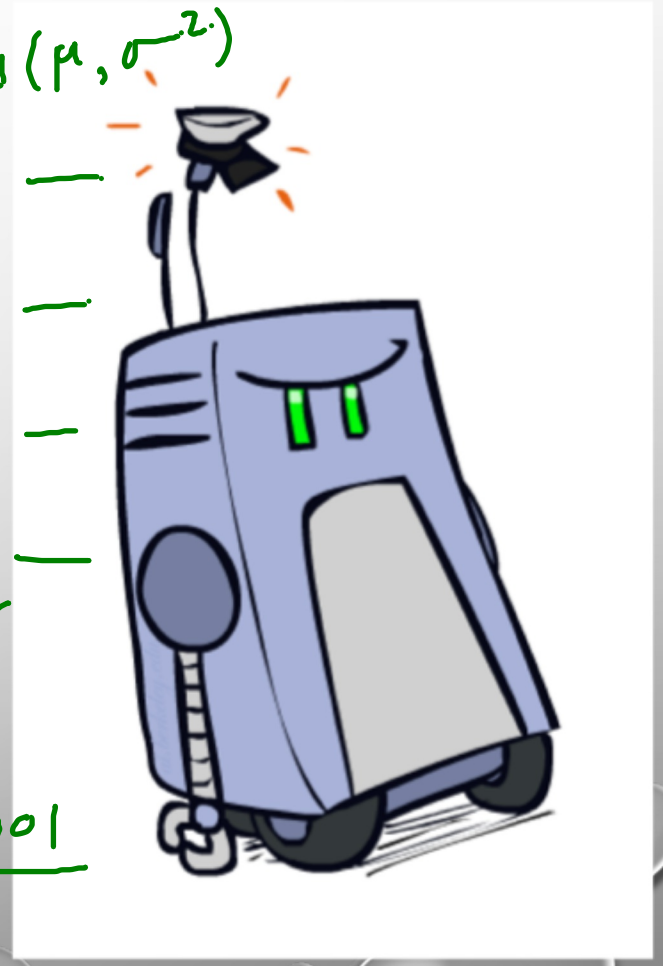
$P(\text{off}|C = 3) = 0.7$

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

0

0.0001

$N(\mu, \sigma^2)$



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?

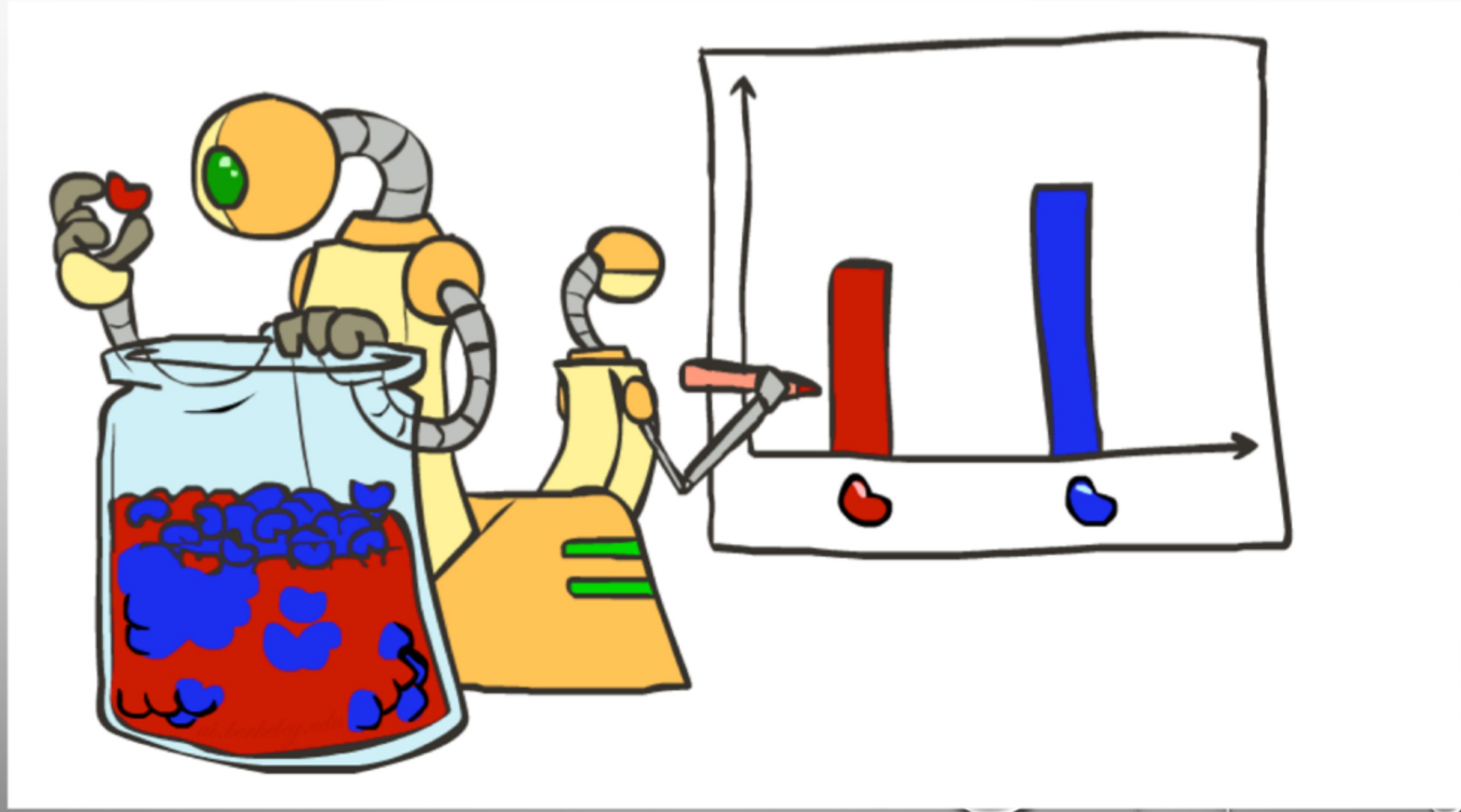
Generalization and Overfitting

- 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

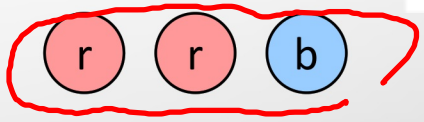
Parameter Estimation



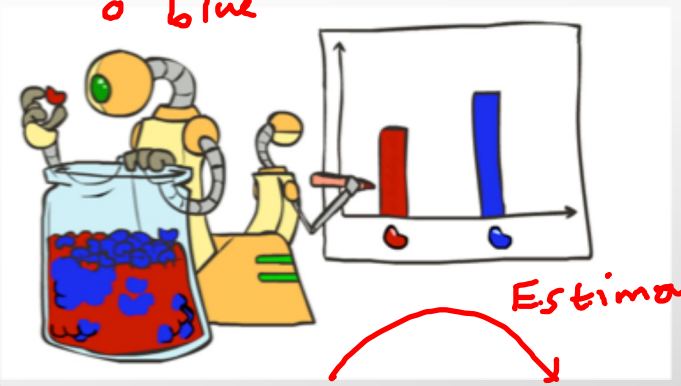
Parameter Estimation

- 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:

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



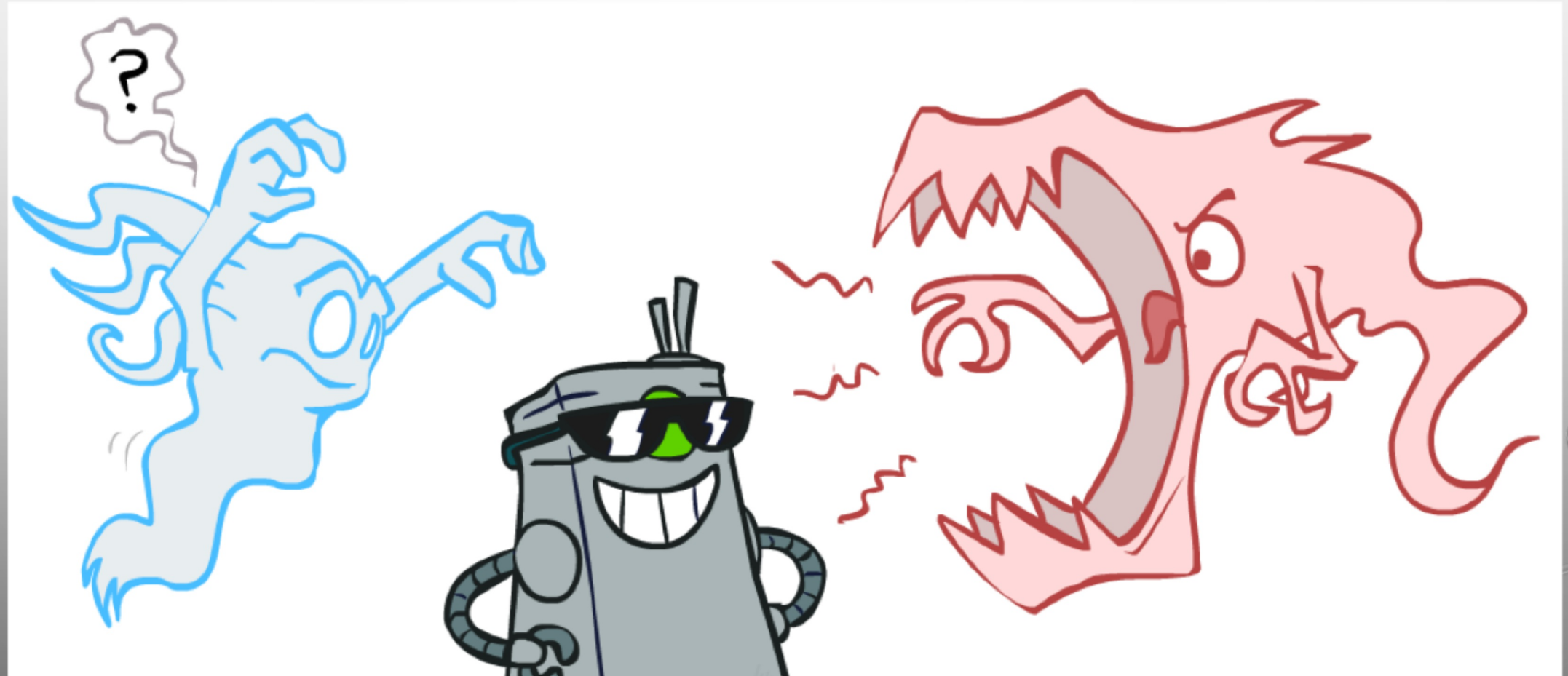
$P_{\text{ML}}(\text{r}) = 2/3$



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

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

Smoothing



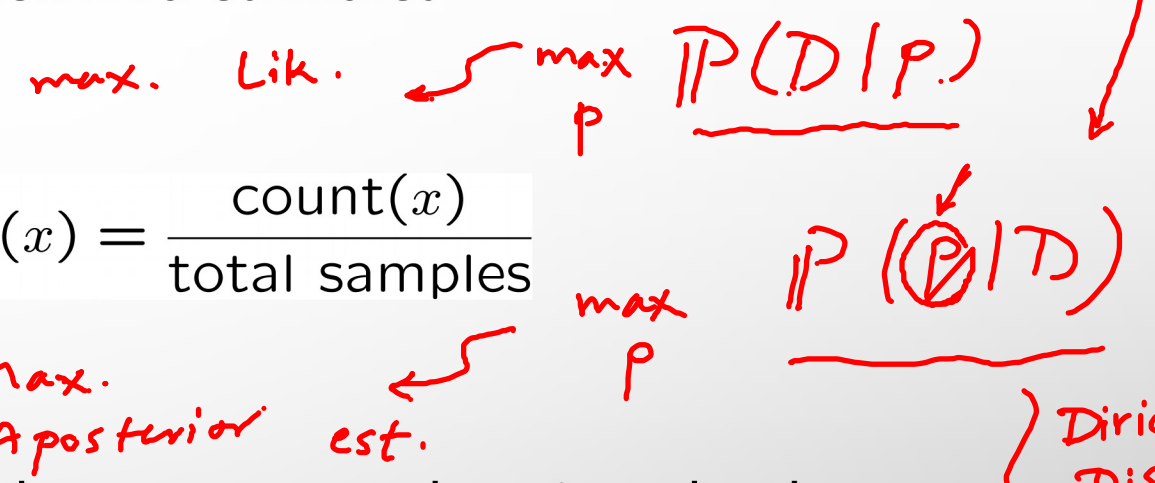
Maximum Likelihood?

- Relative frequencies are the maximum likelihood estimates

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

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

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



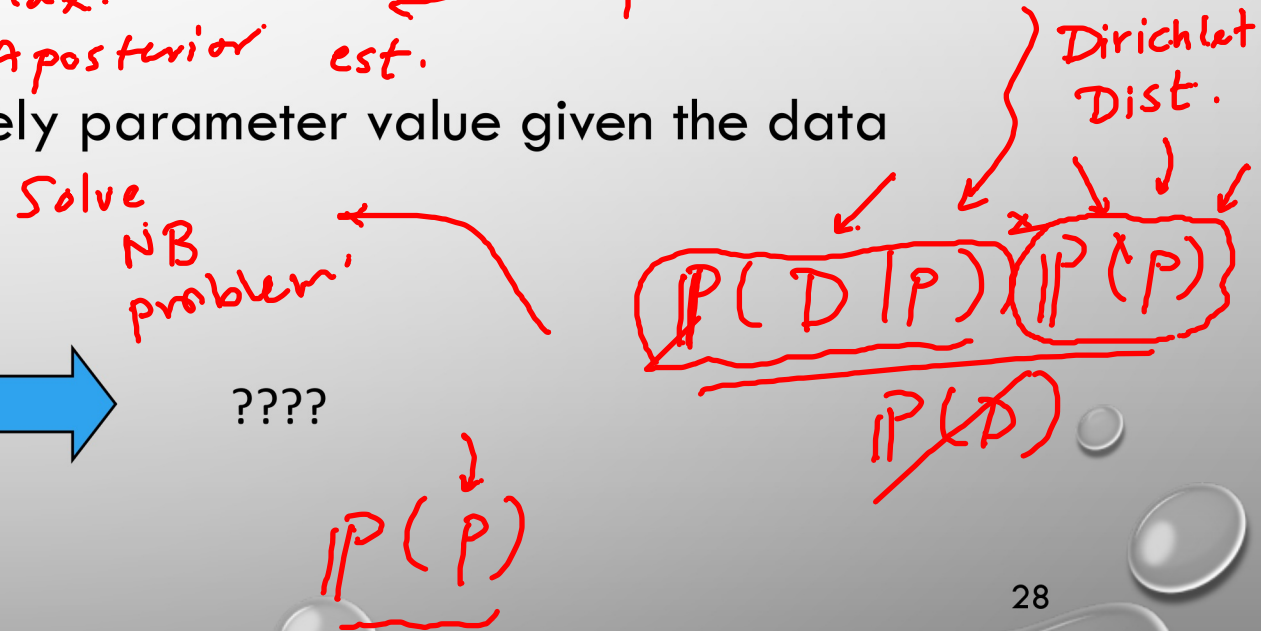
- Another option is to consider the most likely parameter value given the data

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

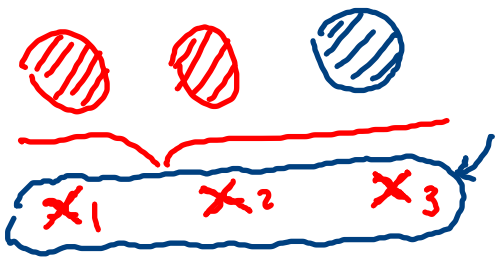
$$= \arg\max_{\theta} P(\mathbf{X}|\theta)P(\theta)/P(\mathbf{X})$$

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

$$\Rightarrow$$????



problem Def.



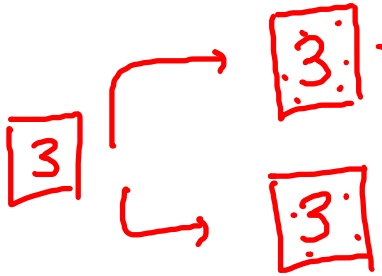
$x_i = 1$ if red

0 if blue

$X_1 \cdots X_n \overset{iid}{\sim}$ Bernoulli(p)

$p = \mathbb{P}(\text{red})$

$1-p = \mathbb{P}(\text{blue})$



Estimation:

$g(X_1 \cdots X_n) =: \hat{p}$

unknown param.

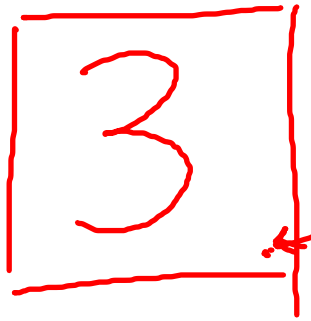
$\max_p \mathbb{P}(D \mid p)$

↳ Maximum Likelihood

* In practice \ and also in theory

if $|D| \to \infty$, $\hat{p} \xrightarrow{p} p$.

* What if $|D|$ is small.



(unseen events)

Sol.

(1) increase traing set size

(2) Augment the data set.

(3) Bayesian Est.

ML. $\mathbb{P}(X_i = x_i \mid p) = p^{x_i}(1-p)^{1-x_i}$

$$\mathbb{P}(D \mid p) = \prod_{i=1}^{n} \mathbb{P}(X_i = x_i \mid p)$$

$$\log \mathbb{P}(D \mid p) = \sum_{i=1}^{n} \mathbb{P}(X_i = x_i \mid p)$$

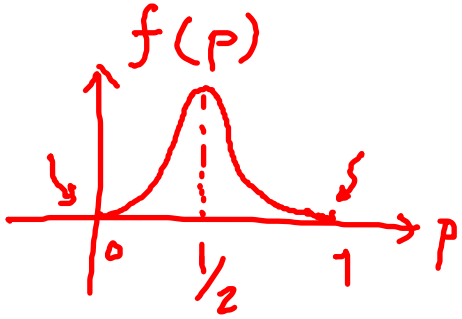
$$= \sum_{i=1}^{n} x_i \log p + (1-x_i) \log 1-p$$

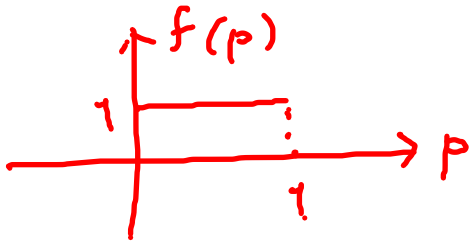
$$\frac{\partial}{\partial p} \log \mathbb{P}(D \mid p) = \sum_{i=1}^{n} \frac{x_i}{p} - \frac{(1-x_i)}{1-p} = 0$$

$$\Rightarrow \hat{p}_{ML} = 1/n \sum_{i=1}^{n} x_i$$

prior dist.

$P(p)$ ⇝





$P(D|p)$ vs. $P(p|D)$ is a better choice, as it makes more sense to pick the most probable unknown!

$$P(p|D) = \frac{P(D|p)\,P(p)}{P(D)}$$

likelihood · Prior · Evidence

$$\hat{p}_{MAP} = \underset{p}{\operatorname{argmax}}\; P(D|p)\,P(p) \rightarrow \hat{p}_{MAP} \overset{?}{=} \hat{p}_{ML}$$

Dirichlet Dist.

$\underline{p} = (p_1, p_2, \cdots, p_K) \rightarrow \sum_{i=1}^{k} p_i = 1$

unknown

$\alpha = 1 \Leftrightarrow k = 0$

$f(\underline{p}) := \frac{1}{Z} \prod_{i=1}^{K} p_i^{\alpha_i - 1}$

params of the Dirichlet

number of colors

$\underline{p} = (p, 1-p)$ $\quad \alpha_1 = \alpha_2 = 2$

$$\left[\prod_{i=1}^{n} p^{x_i} (1-p)^{1-x_i} \right] \cdot \left[p \cdot (1-p) \right] = p^{\sum x_i + 1} (1-p)^{n - \sum x_i + 1}$$

likelihood $\quad$ "conjugate prior"

$P(D|p) \quad P(p)$

likelihood has the same "form" as the posterior

$$\hat{p}_{MAP} = \frac{\sum x_i + 1}{n + 2}$$

Laplace Smoothing

$K \rightarrow \infty \quad \hat{p}_{MAP} = 1/2$

$2K$

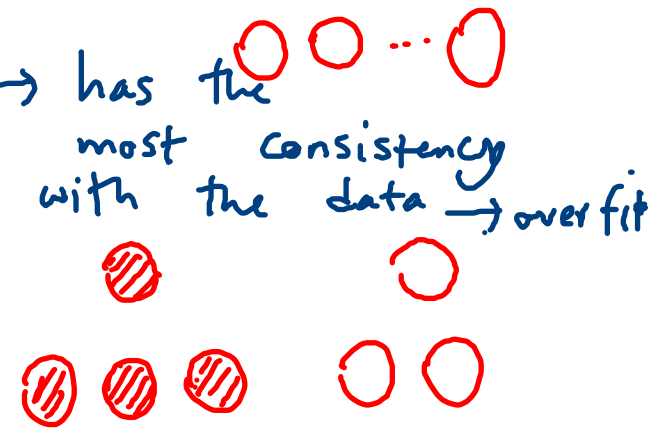
$K \rightarrow$ hyperparam $\rightarrow$ tune

val. data

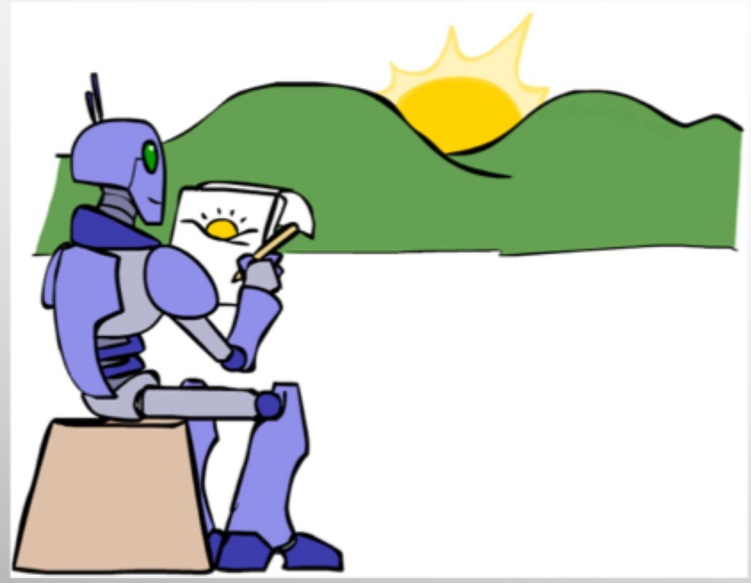
$K \in \{0, 1, 2, \cdots, 10\}$

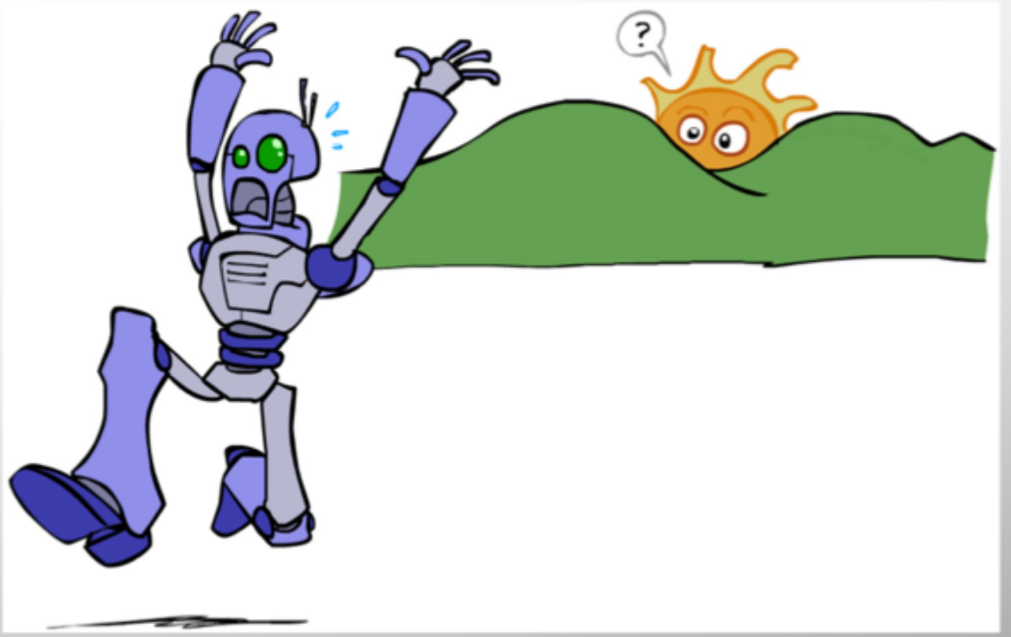
traing data

$\hookrightarrow K = 0 \rightarrow$ has the most consistency with the data $\rightarrow$ overfit



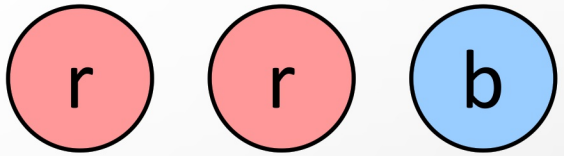
Unseen Events





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

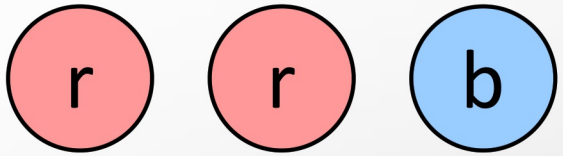
- Laplace's estimate (extended):
  - Pretend you saw every outcome k extra times

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

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

- Laplace for conditionals:
  - Smooth each condition independently:

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



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

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

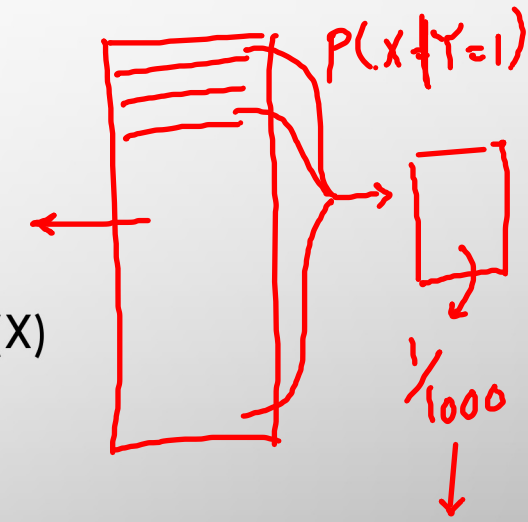
$P_{LAP,100}(X) =$

Estimation: Linear Interpolation

- In practice, Laplace often performs poorly for P(X|Y):
  - When |X| is very large
  - When |Y| is very large
- Another option: linear interpolation
  - Also get the empirical P(X) from the data
  - Make sure the estimate of P(X|Y) isn't too different from the empirical P(X)

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

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



Real NB: Smoothing

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

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

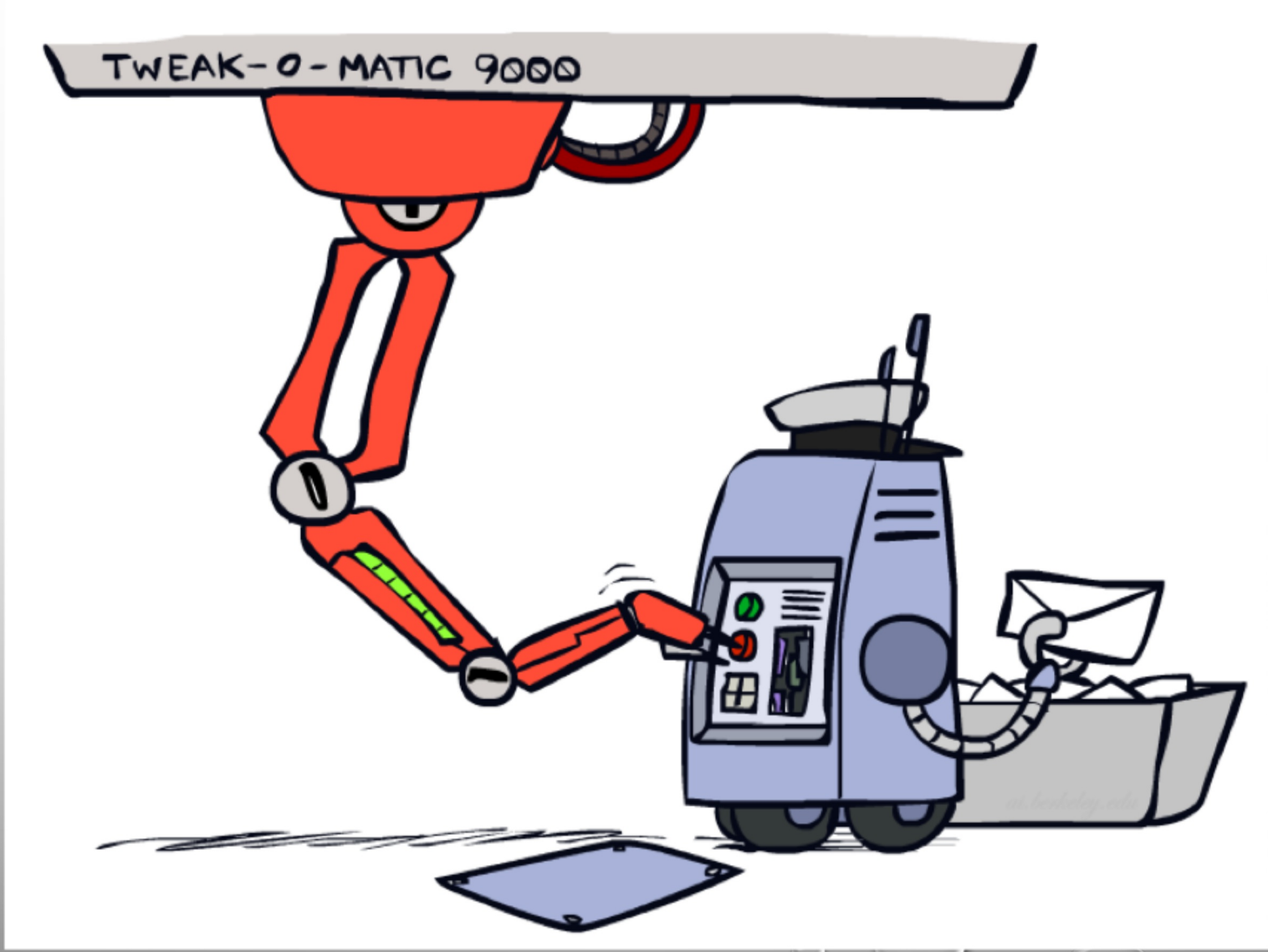
```
helvetica : 11.4
seems     : 10.8
group     : 10.2
ago       :  8.4
areas     :  8.3
...
```

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

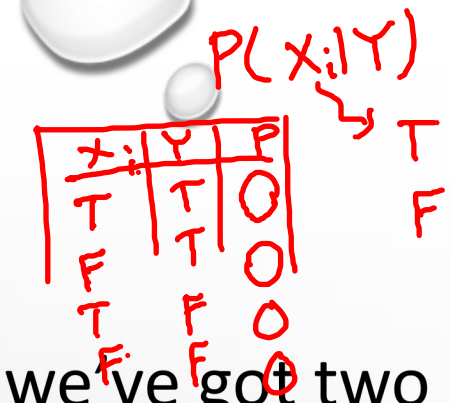
```
verdana : 28.8
Credit  : 28.4
ORDER   : 27.2
<FONT>  : 26.9
money   : 26.5
...
```

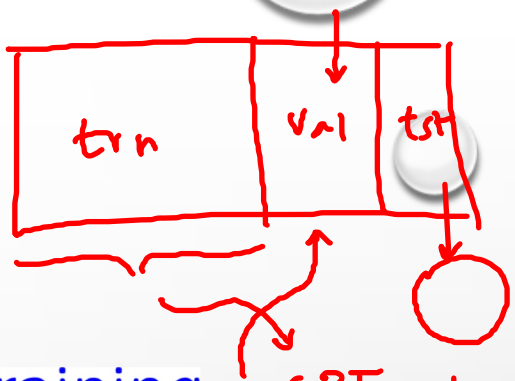
Do these make more sense?

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