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
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
  - ...

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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.
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
- ...

![Image of digit recognition example with labeled numbers 0, 1, 2, and ?]
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.
    \[ \{F_{0,0} = 0, F_{0,1} = 0, F_{0,2} = 1, F_{0,3} = 1, F_{0,4} = 0, \ldots F_{15,15} = 0\} \]
  - 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

\[ P(Y) \]

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<tr>
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<td>0.1</td>
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\[ P(F_{3,1} = \text{on}|Y) \]

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<td>0.05</td>
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\[ P(F_{5,5} = \text{on}|Y) \]

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<td>0.90</td>
<td>0.25</td>
<td>0.85</td>
<td>0.60</td>
<td>0.80</td>
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A general Naïve Bayes model:

\[ P(Y, F_1 \ldots F_n) = P(Y) \prod_{i} P(F_i|Y) \]

- We only have to specify how each feature depends on the class
- Total number of parameters is \textit{linear} in \( n \)
- Model is very simplistic, but often works anyway
Goal: compute posterior distribution over label variable $Y$

- Step 1: get joint probability of label and evidence for each label

\[
P(Y, f_1 \ldots f_n) = \begin{bmatrix} P(y_1, f_1 \ldots f_n) \\ P(y_2, f_1 \ldots f_n) \\ \vdots \\ P(y_k, f_1 \ldots f_n) \\ P(y_k, f_1 \ldots f_n) \end{bmatrix}
\]

- Step 2: sum to get probability of evidence

\[
P(f_1 \ldots f_n) = \frac{P(y_1) \prod_i P(f_i|y_1) + P(y_2) \prod_i P(f_i|y_2) + \cdots + P(y_k) \prod_i P(f_i|y_k)}{P(y_1) + P(y_2) + \cdots + P(y_k)}
\]

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

\[
P(Y|f_1 \ldots f_n) = \frac{P(Y, f_1 \ldots f_n)}{P(f_1 \ldots f_n)}
\]
A Spam Filter

- Naïve Bayes spam filter
- Data:
  - Collection of emails, labeled spam or ham
  - Note: someone has to hand label all this data!
  - Split into training, held-out, test sets
- Classifiers
  - Learn on the training set
  - (Tune it on a held-out set)
  - Test it on new emails

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Naïve Bayes for Text

- Bag-of-words Naïve Bayes:
  - Features: \( W_i \) is the word at 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:
  \[
P(Y, W_1 \ldots W_n) = P(Y) \prod_i P(W_i|Y)
\]

- “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

Word at position \( i \), not \( i^{th} \) word in the dictionary!

Oh sorry I was still on mute
Example: Spam Filtering

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

| \( P(Y) \) | \( P(W|\text{spam}) \) | \( P(W|\text{ham}) \) |
|----------------|----------------|----------------|
| ham : 0.66     | the : 0.0156   | the : 0.0210   |
| spam: 0.33     | to : 0.0153    | to : 0.0133    |
|                 | and : 0.0115   | of : 0.0119    |
|                 | of : 0.0095    | 2002: 0.0110   |
|                 | you : 0.0093   | with: 0.0110   |
|                 | a : 0.0086     | from: 0.0108   |
|                 | with: 0.0080   | and : 0.0107   |
|                 | from: 0.0075   | a : 0.0105     |
|                 | ...            | ...            |
## Spam Example

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

- $P(Y)$
- $P(W_1|Y)$
- $P(W_2|Y)$
- ...
- ...
- ...
- ...
- ...
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 \( P(Y|F_1...F_n) \)
  - 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
Parameter Estimation
Parameter Estimation with Maximum Likelihood

- 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:
    \[
P_{\text{ML}}(x) = \frac{\text{count}(x)}{\text{total samples}}
    \]
  - This is the estimate that maximizes the *likelihood of the data*
    \[
    L(x, \theta) = \prod_i P_\theta(x_i) = \theta \cdot (1 - \theta)
    \]
- $P_{\text{ML}}(r) = 2/3$
- $P_\theta(x = \text{red}) = \theta$
- $P_\theta(x = \text{blue}) = 1 - \theta$
Parameter Estimation with Maximum Likelihood

- **Data:** Observed set $D$ of $\alpha_H$ Heads and $\alpha_T$ Tails
- **Hypothesis space:** Binomial distributions
- **Learning:** finding $\theta$ is an optimization problem
  - What’s the objective function?
    \[ P(D \mid \theta) = \theta^{\alpha_H} (1 - \theta)^{\alpha_T} \]
- **MLE:** Choose $\theta$ to maximize probability of $D$
  \[ \hat{\theta} = \arg \max_{\theta} P(D \mid \theta) \]
  \[ = \arg \max_{\theta} \ln P(D \mid \theta) \]
Parameter Estimation with Maximum Likelihood

\[ \hat{\theta} = \arg \max_\theta \ln P(D | \theta) \]
\[ = \arg \max_\theta \ln \theta^{\alpha_H} (1 - \theta)^{\alpha_T} \]

- Set derivative to zero, and solve!

\[ \frac{d}{d\theta} \ln P(D | \theta) = \frac{d}{d\theta} [\ln \theta^{\alpha_H} (1 - \theta)^{\alpha_T}] \]
\[ = \frac{d}{d\theta} [\alpha_H \ln \theta + \alpha_T \ln(1 - \theta)] \]
\[ = \alpha_H \frac{d}{d\theta} \ln \theta + \alpha_T \frac{d}{d\theta} \ln(1 - \theta) \]
\[ = \frac{\alpha_H}{\theta} - \frac{\alpha_T}{1 - \theta} = 0 \]
\[ \hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T} \]
Parameter Estimation with Maximum Likelihood

- How do we estimate the conditional probability tables?
  - Maximum Likelihood, which corresponds to counting

- Need to be careful though ... let’s see what can go wrong..
Underfitting and Overfitting
Example: Overfitting

\[ P(\text{features}, C = 2) \]
\[ P(C = 2) = 0.1 \]
\[ P(\text{on}|C = 2) = 0.8 \]
\[ P(\text{on}|C = 2) = 0.1 \]
\[ P(\text{off}|C = 2) = 0.1 \]
\[ P(\text{on}|C = 2) = 0.01 \]

\[ P(\text{features}, C = 3) \]
\[ P(C = 3) = 0.1 \]
\[ P(\text{on}|C = 3) = 0.8 \]
\[ P(\text{on}|C = 3) = 0.9 \]
\[ P(\text{off}|C = 3) = 0.7 \]
\[ P(\text{on}|C = 3) = 0.0 \]

2 wins!!
Example: Overfitting

- relative probabilities (odds ratios):

\[
\frac{P(W|\text{ham})}{P(W|\text{spam})} \quad \text{and} \quad \frac{P(W|\text{spam})}{P(W|\text{ham})}
\]

| South-west : inf | Screens : inf |
| Nation : inf | Minute : inf |
| Morally : inf | Guaranteed : inf |
| Nicely : inf | $205.00 : inf |
| Extent : inf | Delivery : inf |
| Seriously : inf | Signature : inf |
| ... | ... |

What went wrong here?
Overfitting

Degree 15 polynomial
Training and Testing
Important Concepts

- **Data:** labeled instances, e.g. emails marked spam/ham
  - Training set
  - Held out set
  - Test set

- **Features:** attribute-value pairs which characterize each x

- **Experimentation cycle**
  - Learn parameters (e.g. model probabilities) on training set
  - (Tune hyperparameters on held-out set)
  - Compute accuracy on test set
  - Very important: never “peek” at the test set!

- **Evaluation**
  - Accuracy: fraction of instances predicted correctly

- **Overfitting and generalization**
  - Want a classifier which does well on test data
  - **Overfitting:** fitting the training data very closely, but not generalizing well
  - **Underfitting:** fits the training set poorly
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
Laplace Smoothing

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

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

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

\[
P_{ML}(X) = \quad P_{LAP}(X) =
\]
Laplace Smoothing

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

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

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

- Laplace for conditionals:
  - Smooth each condition independently:

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

  $P_{LAP,0}(X) =$
  $P_{LAP,1}(X) =$
  $P_{LAP,100}(X) =$
Laplace Smoothing Can Be More Formally Derived

- Relative frequencies are the maximum likelihood estimates

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

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

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

\[
\theta_{MAP} = \arg \max_\theta P(\theta|X) = \arg \max_\theta P(X|\theta)P(\theta)/P(X)
\]

\[
= \arg \max_\theta P(X|\theta)P(\theta)
\]

"right" choice of \(P(\theta)\)

\(-\) Laplace estimates
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 $\alpha$ is 0? 1?

- For even better ways to estimate parameters, as well as details of the math, see cs281a, cs288
Real NB: Smoothing

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

\[
\frac{P(W|\text{ham})}{P(W|\text{spam})} \quad \text{and} \quad \frac{P(W|\text{spam})}{P(W|\text{ham})}
\]

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<tr>
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<tr>
<td>group</td>
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<tr>
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<tr>
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Do these make more sense?
Tuning
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
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
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