Machine Learning

- Up until now: how to reason in a model and how to make optimal decisions

- Machine learning: how to select a model on the basis of data / experience
  - Learning parameters (e.g. probabilities)
  - Learning structure (e.g. BN graphs)
  - Learning hidden concepts (e.g. clustering)
Example: Spam Filter

- **Input:** 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

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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
  - ...

<table>
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<tr>
<th>0</th>
<th>1</th>
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Other Classification Tasks

- In classification, we predict labels $y$ (classes) for inputs $x$

- Examples:
  - Spam detection (input: document, classes: spam / ham)
  - OCR (input: images, classes: characters)
  - Medical diagnosis (input: symptoms, classes: diseases)
  - Automatic essay grader (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!
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
Bayes Nets for Classification

- One method of classification:
  - Use a probabilistic model!
  - Features are observed random variables $F_i$
  - $Y$ is the query variable
  - Use probabilistic inference to compute most likely $Y$

$$y = \arg\max_y P(y|f_1 \ldots f_n)$$

- You already know how to do this inference
Simple Classification

- Simple example: two binary features

\[
P(m|s, f) \quad \text{direct estimate}
\]

\[
P(m|s, f) = \frac{P(s, f|m)P(m)}{P(s, f)}
\]

\[
P(m|s, f) = \frac{P(s|m)P(f|m)P(m)}{P(s, f)}
\]

Bayes estimate (no assumptions)

Conditional independence

\[
\begin{align*}
P(m, s, f) &= P(s|m)P(f|m)P(m) \\
P(\bar{m}, s, f) &= P(s|\bar{m})P(f|\bar{m})P(\bar{m})
\end{align*}
\]
A general naive Bayes model:

\[ P(Y, F_1 \ldots F_n) = P(Y) \prod_i P(F_i | Y) \]

- We only specify how each feature depends on the class
- Total number of parameters is linear in n
Inference for Naïve Bayes

- **Goal: compute posterior over causes**
  - Step 1: get joint probability of causes and evidence
  \[
  P(Y, f_1 \ldots f_n) = \\
  \begin{bmatrix}
  P(y_1, f_1 \ldots f_n) \\
  P(y_2, f_1 \ldots f_n) \\
  \vdots \\
  P(y_k, f_1 \ldots f_n)
  \end{bmatrix}
  \]
  \[
  = \\
  \begin{bmatrix}
  P(f_1) \prod_i P(f_i|c_1) \\
  P(f_2) \prod_i P(f_i|c_2) \\
  \vdots \\
  P(f_k) \prod_i P(f_i|c_k)
  \end{bmatrix}
  \]
  \[
  \frac{P(f_1 \ldots f_n)}{P(Y|f_1 \ldots f_n)}
  \]
  
  - Step 2: get probability of evidence
  
  - Step 3: renormalize
General Naïve Bayes

- What do we need in order to use naïve Bayes?

  - Inference (you know this part)
    - Start with a bunch of conditionals, 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: we’ll look at this now
A Digit Recognizer

- Input: pixel grids
- Output: a digit 0-9
Naïve Bayes for Digits

- **Simple version:**
  - One feature $F_{ij}$ for each grid position $<i,j>$
  - Possible 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.
    \[ \langle F_{0,0} = 0, F_{0,1} = 0, F_{0,2} = 1, F_{0,3} = 1, F_{0,4} = 0, \ldots F_{15,15} = 0 \rangle \]
  - Here: lots of features, each is binary

- **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?
Examples: CPTs

\[ P(Y) \]

\[
\begin{array}{c|c}
1 & 0.1 \\
2 & 0.1 \\
3 & 0.1 \\
4 & 0.1 \\
5 & 0.1 \\
6 & 0.1 \\
7 & 0.1 \\
8 & 0.1 \\
9 & 0.1 \\
0 & 0.1 \\
\end{array}
\]

\[ P(F_{3,1} = on|Y) \]

\[
\begin{array}{c|c}
1 & 0.01 \\
2 & 0.05 \\
3 & 0.05 \\
4 & 0.30 \\
5 & 0.80 \\
6 & 0.90 \\
7 & 0.05 \\
8 & 0.60 \\
9 & 0.50 \\
0 & 0.80 \\
\end{array}
\]

\[ P(F_{5,5} = on|Y) \]

\[
\begin{array}{c|c}
1 & 0.05 \\
2 & 0.01 \\
3 & 0.90 \\
4 & 0.80 \\
5 & 0.90 \\
6 & 0.90 \\
7 & 0.25 \\
8 & 0.85 \\
9 & 0.60 \\
0 & 0.80 \\
\end{array}
\]
Parameter Estimation

- Estimating distribution of random variables like $X$ or $X \mid Y$

- *Empirically*: use training data
  - For each outcome $x$, look at the *empirical rate* of that value:
    $$P_{ML}(x) = \frac{\text{count}(x)}{\text{total samples}}$$
    $$P_{ML}(r) = 1/3$$
  - This is the estimate that maximizes the *likelihood of the data*
    $$L(x, \theta) = \prod_i P_\theta(x_i)$$

- *Elicitation*: ask a human!
  - Usually need domain experts, and sophisticated ways of eliciting probabilities (e.g. betting games)
  - Trouble calibrating
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:**
  - Predict unknown class label (spam vs. ham)
  - Assume evidence features (e.g. the words) are independent
  - Warning: subtly different assumptions than before!

- **Generative model**
  \[
P(C, W_1 \ldots W_n) = P(Y) \prod_i P(W_i|C)\]

- **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 \(P(W|C)\)
    - Why make this assumption?
Example: Spam Filtering

- **Model:** \[ P(C, W_1 \ldots W_n) = P(C') \prod_{i} P(W_i|C') \]

- **What are the parameters?**

|       | \( P(C) \)          | \( P(W|\text{spam}) \)                                      | \( P(W|\text{ham}) \)         |
|-------|----------------------|-------------------------------------------------------------|-----------------------------|
| **ham** | 0.66                 | \begin{tabular}{c} the : 0.0156 \\ to : 0.0153 \\ and : 0.0115 \\ of : 0.0095 \\ you : 0.0093 \\ a : 0.0086 \\ with : 0.0080 \\ from : 0.0075 \\ ... \end{tabular} | \begin{tabular}{c} the : 0.0210 \\ to : 0.0133 \\ of : 0.0119 \\ 2002 : 0.0110 \\ with : 0.0108 \\ from : 0.0107 \\ and : 0.0105 \\ a : 0.0100 \\ ... \end{tabular} |
| **spam** | 0.33                 |                                                             |                             |

- **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    |

$P(\text{spam} \mid w) = 98.9$
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: Spam Filtering

- Raw probabilities alone don’t affect the posteriors; relative probabilities (odds ratios) do:

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

| 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?
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
Estimation: Smoothing

- **Problems with maximum likelihood estimates:**
  - If I flip a coin once, and it’s heads, what’s the estimate for $P(\text{heads})$?
  - What if I flip 10 times with 8 heads?
  - What if I flip 10M times with 8M heads?

- **Basic idea:**
  - We have some prior expectation about parameters (here, the probability of heads)
  - Given little evidence, we should skew towards our prior
  - Given a lot of evidence, we should listen to the data
Estimation: Smoothing

- Relative frequencies are the maximum likelihood estimates

\[
\theta_{ML} = \arg \max_{\theta} P(X|\theta) = \arg \max_{\theta} \prod_{i} P_\theta(X_i) \quad \Rightarrow \quad P_{ML}(x) = \frac{\text{count}(x)}{\text{total samples}}
\]

- In Bayesian statistics, we think of the parameters as just another random variable, with its own distribution

\[
\theta_{MAP} = \arg \max_{\theta} P(\theta|X) = \arg \max_{\theta} P(X|\theta)P(\theta)/P(X) = \arg \max_{\theta} P(X|\theta)P(\theta)
\]
Estimation: 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 as a MAP estimate with *Dirichlet priors* (see cs281a)

  \[
  P_{ML}(X) = \\
  P_{LAP}(X) =
  \]
Estimation: 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 $P(X)$ from the data
  - Make sure the estimate of $P(X|Y)$ isn’t too different from $P(X)$

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

- 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:

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

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</tr>
<tr>
<td>group</td>
<td>10.2</td>
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<tr>
<td>ago</td>
<td>8.4</td>
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<tr>
<td>areas</td>
<td>8.3</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
</tbody>
</table>

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

*Do these make more sense?*
Tuning on Held-Out Data

- Now we’ve got two kinds of unknowns
  - Parameters: the probabilities $P(Y|X)$, $P(Y)$
  - Hyperparameters, like the amount of smoothing to do: $k$, $\alpha$

- Where to learn?
  - Learn parameters from training data
  - Must 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
Baselines

- **First task: 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

- 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
    \[ \text{confidence}(x) = \arg \max_y P(y|x) \]
  - 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?
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
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
Case-Based Reasoning

- Similarity for classification
  - Case-based reasoning
  - Predict an instance’s label using similar instances

- Nearest-neighbor classification
  - 1-NN: copy the label of the most similar data point
  - K-NN: let the k nearest neighbors vote (have to devise a weighting scheme)
  - Key issue: how to define similarity
  - Trade-off:
    - Small k gives relevant neighbors
    - Large k gives smoother functions
  - Sound familiar?

- [DEMO]

http://www.cs.cmu.edu/~zhuxj/courseproject/knndemo/KNN.html
Recap: Nearest-Neighbor

- **Nearest neighbor:**
  - Classify test example based on closest training example
  - Requires a similarity function (kernel)
  - **Eager learning:** extract classifier from data
  - **Lazy learning:** keep data around and predict from it at test time

<table>
<thead>
<tr>
<th>Truth</th>
<th>2 Examples</th>
<th>10 Examples</th>
<th>100 Examples</th>
<th>10000 Examples</th>
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</table>

Examples 10 Examples 100 Examples 10000 Examples
Nearest-Neighbor Classification

- Nearest neighbor for digits:
  - Take new image
  - Compare to all training images
  - Assign based on closest example

- Encoding: image is vector of intensities:
  \[ \mathbf{1} = \langle 0.0, 0.0, 0.3, 0.8, 0.7, 0.1, \ldots, 0.0 \rangle \]

- What’s the similarity function?
  - Dot product of two images vectors?
    \[ \text{sim}(x, y) = x \cdot y = \sum_{i} x_i y_i \]
    - Usually normalize vectors so \( ||x|| = 1 \)
    - \( \text{min} = 0 \) (when?), \( \text{max} = 1 \) (when?)