CPSC 340: Machine Learning and Data Mining

Probabilistic Classification Fall 2017

Admin

- Assignment 0 is due tonight: you should be almost done.
 1 late day to hand it in Monday, 2 late days for Wednesday.
- Assignment 1 is coming Monday: start early.

- Important webpages:
 - www.cs.ubc.ca/~schmidtm/Courses/340-F17
 - www.piazza.com/ubc.ca/winterterm12017/cpsc340/home

Last Time: Training, Testing, and Validation

• Training step:

• Prediction step:

Inputi set of '(' testing examples
$$\tilde{x}_i$$
 and a model.
Output predictions \hat{y}_i for the testing examples.

- What we are interested in is the test error:
 - Error made by prediction step on new data.

Last Time: Fundamental Trade-Off

• We decomposed test error to get a fundamental trade-off:



– Training error goes down as a decision tree gets deeper.

- But E_{approxr} goes up as model gets complicated:
 - Training error becomes a worse approximation of test error.

Last Time: Validation Errorr

- Golden rule: we can't look at test data during training.
- But we can approximate E_{test} with a validation error:
 - Error on a set of training examples we "hid" during training.



- Find the decision tree based on the "train" rows.
- Validation error is the error of the decision tree on the "validation" rows.

- Scenario 1:
 - "I built a model based on the data you gave me."
 - "It classified your data with 98% accuracy."
 - "It should get 98% accuracy on the rest of your data."
- Probably not:
 - They are reporting training error.
 - This might have nothing to do with test error.
 - E.g., they could have fit a very deep decision tree.
- Why 'probably'?
 - If they only tried a few very simple models, the 98% might be reliable.
 - E.g., they only considered decision stumps with simple 1-variable rules.

- Scenario 2:
 - "I built a model based on half of the data you gave me."
 - "It classified the other half of the data with 98% accuracy."
 - "It should get 98% accuracy on the rest of your data."
- Probably:
 - They computed the validation error once.
 - This is an unbiased approximation of the test error.
 - Trust them if you believe they didn't violate the golden rule.

- Scenario 3:
 - "I built 10 models based on half of the data you gave me."
 - "One of them classified the other half of the data with 98% accuracy."
 - "It should get 98% accuracy on the rest of your data."
- Probably:
 - They computed the validation error a small number of times.
 - Maximizing over these errors is a biased approximation of test error.
 - But they only maximized it over 10 models, so bias is probably small.
 - They probably know about the golden rule.

- Scenario 4:
 - "I built 1 billion models based on half of the data you gave me."
 - "One of them classified the other half of the data with 98% accuracy."
 - "It should get 98% accuracy on the rest of your data."
- Probably not:
 - They computed the validation error a huge number of times.
 - Maximizing over these errors is a biased approximation of test error.
 - They tried so many models, one of them is likely to work by chance.
- Why 'probably'?
 - If the 1 billion models were all extremely-simple, 98% might be reliable.

- Scenario 5:
 - "I built 1 billion models based on the first third of the data you gave me."
 - "One of them classified the second third of the data with 98% accuracy."
 - "It also classified the last third of the data with 98% accuracy."
 - "It should get 98% accuracy on the rest of your data."
- Probably:
 - They computed the first validation error a huge number of times.
 - But they had a second validation set that they only looked at once.
 - The second validation set gives unbiased test error approximation.
 - This is ideal, as long as they didn't violate golden rule on the last third.
 - And assuming you are using IID data in the first place.

Validation Error and Optimization Bias

- Optimization bias is small if you only compare a few models:
 - Best decision tree on the training set among depths, 1, 2, 3,..., 10.
 - Risk of overfitting to validation set is low if we try 10 things.
- Optimization bias is large if you compare a lot of models:
 - All possible decision trees of depth 10 or less.
 - Here we're using the validation set to pick between a billion+ models:
 - Risk of overfitting to validation set is high: could have low validation error by chance.
 - If you did this, you might want a second validation set to detect overfitting.

Cross-Validation (CV)

- Isn't it wasteful to only use part of your data?
- 5-fold cross-validation:
 - Train on 80% of the data, validate on the other 20%.
 - Repeat this 5 more times with different splits, and average the score.

$$X = \begin{bmatrix} & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & &$$

Cross-Validation (CV)

- You can take this idea further:
 - 10-fold cross-validation: train on 90% of data and validate on 10%.
 - Repeat 10 times and average.
 - Leave-one-out cross-validation: train on all but one training example.
 - Repeat n times and average.
- Gets more accurate but more expensive with more folds.
 - To choose depth we compute the cross-validation score for each depth.
- As before, if data is ordered then folds should be random splits.
 Randomize first, then split into fixed folds.

Cross-Validation Pseudo-Code

(pause)

/

The "Best" Machine Learning Model

- Decision trees are not always most accurate on test error.
- What is the "best" machine learning model?
- First we need to define generalization error:
 - Test error restricted to new feature combinations (no x_i from train set).
- No free lunch theorem:
 - There is **no** "best" model achieving the best generalization error for every problem.
 - If model A generalizes better to new data than model B on one dataset, there is another dataset where model B works better.
- This question is like asking which is "best" among "rock", "paper", and "scissors".

The "Best" Machine Learning Model

- Implications of the lack of a "best" model:
 - We need to learn about and try out multiple models.
- So which ones to study in CPSC 340?
 - We'll usually motivate each method by a specific application.
 - But we're focusing on models that have been effective in many applications.
- Caveat of no free lunch (NFL) theorem:
 - The world is very structured.
 - Some datasets are more likely than others.
 - Model A really could be better than model B on every real dataset in practice.
- Machine learning research:
 - Large focus on models that are useful across many applications.

Application: E-mail Spam Filtering

- Want a build a system that detects spam e-mails.
 - Context: spam used to be a big problem.

		_	to se
Jannie Keenan	ualberta You are owed \$24,718.11	A	Be o
Abby	ualberta USB Drives with your Logo		Hey
Rosemarie Page	Re: New request created with ID: ##62		Do y Are solu
Shawna Bulger	RE: New request created with ID: ##63		We sinc
Gary	ualberta Cooperation		Plea Lam servi
			Best



• Can we formulate as supervised learning?

Spam Filtering as Supervised Learning

• Collect a large number of e-mails, gets users to label them.

\$	Hi	CPSC	340	Vicodin	Offer	•••	Spam?
1	1	0	0	1	0		1
0	0	0	0	1	1		1
0	1	1	1	0	0		0

- We can use $(y_i = 1)$ if e-mail 'i' is spam, $(y_i = 0)$ if e-mail is not spam.
- Extract features of each e-mail (like bag of words).

- $(x_{ij} = 1)$ if word/phrase 'j' is in e-mail 'i', $(x_{ij} = 0)$ if it is not.

Feature Representation for Spam

- Are there better features than bag of words?
 - We add bigrams (sets of two words):
 - "CPSC 340", "wait list", "special deal".
 - Or trigrams (sets of three words):
 - "Limited time offer", "course registration deadline", "you're a winner".
 - We might include the sender domain:
 - <sender domain == "mail.com">.
 - We might include regular expressions:
 - <your first and last name>.
- Also, note that we only need list of non-zero features for each x_i.

Review of Supervised Learning Notation

• We have been using the notation 'X' and 'y' for supervised learning:



- X is matrix of all features, y is vector of all labels.
 - We use y_i for the label of object 'i' (element 'i' of 'y').
 - We use x_{ii} for feature 'j' of object 'i'.
 - We use x_i as the list of features of object 'i' (row 'i' of 'X').
 - So in the above x₃ = [0 1 1 1 0 0 ...].

Probabilistic Classifiers

- For years, best spam filtering methods used naïve Bayes.
 - A probabilistic classifier based on Bayes rule.
 - It tends to work well with bag of words.
 - Last year shown to improve on state of the art for CRISPR "gene editing" (<u>link</u>).
- Probabilistic classifiers model the conditional probability, $p(y_i | x_i)$.
 - "If a message has words x_i , what is probability that message is spam?"
- Classify it has spam if probability of spam is higher than not spam:
 - If $p(y_i = "spam" | x_i) > p(y_i = "not spam" | x_i)$
 - return "spam".
 - Else
 - return "not spam".

• To model conditional probability, naïve Bayes uses Bayes rule:

$$p(y_i = "spam" | x_i) = p(x_i | y_i = "spam")p(y_i = "spam")$$

 $p(x_i)$

- So we need to figure out three types of terms:
 - Marginal probabilities $p(y_i)$ that an e-mail is spam.
 - Marginal probability $p(x_i)$ that an e-mail has the set of words x_i .
 - Conditional probability $P(x_i | y_i)$ that a spam e-mail has the words x_i .
 - And the same for non-spam e-mails.

$$p(y_i = "spam" | x_i) = p(x_i | y_i = "spam")p(y_i = "spam") p(x_i)$$

• What do these terms mean?



$$p(y_i = "spam" | x_i) = p(x_i | y_i = "spam")p(y_i = "spam") p(x_i)$$

- p(y_i = "spam") is probability that a random e-mail is spam.
 - This is easy to approximate from data: use the proportion in your data.

This is a "maximum likelihood estimate", a concept we'll discuss in detail later. If you're interested in a proof, see <u>here</u>.

$$p(y_i = "spam" | x_i) = p(x_i | y_i = "spam")p(y_i = "spam") p(x_i)$$

- $p(x_i)$ is probability that a random e-mail has features x_i :
 - This is hard to approximate (there are so many possible e-mails).



$$p(y_i = "spam" | x_i) = p(x_i | y_i = "spam")p(y_i = "spam") p(x_i)$$

- $p(x_i)$ is probability that a random e-mail has features x_i :
 - This is hard to approximate (there are so many possible e-mails), but it turns out we can ignore it:

Naive Bayes returns "span" if
$$p(y_i = "span" \mid x_i) > p(y_i = "nt span" \mid x_i)$$
.
By Bayes rule this means $p(x_i \mid y_i = "span")p(y_i = "span") > p(x_i \mid y_i = "not span")dy_i = "ntypi" p(x_i)$
Multiply both sides by $p(x_i)$:
 $p(x_i \mid y_i = "span")p(y_i = "span") > p(x_i \mid y_i = "not span")dy_i = "ntypi"$

$$P(y_i = "spam" | x_i) = \frac{P(x_i | y_i = "spam")P(y_i = "spam")}{P(x_i)}$$

• $p(x_i | y_i = "spam")$ is probability that spam has features x_i .



Naïve Bayes

• Naïve Bayes makes a big assumption to make things easier:

- We assume *all* features x_i are conditionally independent give label y_i.
 - Once you know it's spam, probability of "vicodin" doesn't depend on "CPSC 340".
 - Definitely not true, but sometimes a good approximation.
- And now we only need easy quantities like p("vicodin" = 1 | y_i = "spam").

Naïve Bayes

• p("vicodin" = 1 | "spam" = 1) is probability of seeing "vicodin" in spam.



• Easy to estimate: p(vicodin=1/spam=1)= # spam messages w/vicodin # spam messages

Naïve Bayes

• Naïve Bayes more formally:

• Post-lecture slides: how to train/test by hand on a simple example.

Summary

- Optimization bias: using a validation set too much overfits.
- Cross-validation: allows better use of data to estimate test error.
- No free lunch theorem: there is no "best" ML model.
- Probabilistic classifiers: try to estimate $p(y_i | x_i)$.
- Naïve Bayes: simple probabilistic classifier based on counting.
 - Uses conditional independence assumptions to make training practical.

• Next time:

– A "best" machine learning model as 'n' goes to ∞ .

Naïve Bayes Training Phase

• Training a naïve Bayes model:



Naïve Bayes Training Phase

• Training a naïve Bayes model:

1. Set
$$n_c$$
 to the number of times $(y_i = c)$.










Given a test example
$$\hat{x}_i$$
 we want to find the 'c' maximizing $p(\hat{x}_i | \hat{y}_i = c)$

Under the naive Bayes assumption we can maximize:

$$p(\tilde{y}_{i}=c \mid \tilde{x}_{i}) \propto \prod_{j=1}^{d} \left[p(\tilde{x}_{ij} \mid \tilde{y}_{i}=c) \right] p(\tilde{y}_{i}=c)$$

Given a test example
$$\hat{x}_i$$
, we set production \hat{y}_i to the 'c' maximizing $p(\hat{x}_i | \hat{y}_i = c)$

Under the naive Bayes assumption we can maximize:

$$p(\tilde{y}_{i}=c \mid \tilde{x}_{i}) \propto \prod_{j=1}^{d} \left[p(\tilde{x}_{ij} \mid \tilde{y}_{i}=c) \right] p(\tilde{y}_{i}=c)$$



• Prediction in a naïve Bayes model:

Consider
$$\hat{x}_{i} = [1]$$
 in this data set -9

$$p(\hat{y}_{i}=0 | \hat{x}_{i}) \propto p(\hat{x}_{i}=1 | \hat{y}_{i}=0) p(\hat{x}_{2}=1 | \hat{y}_{i}=0) p(\hat{y}_{i}=0)$$

$$= (1) \qquad (0.25) \qquad (0.4) = 0. \qquad X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad y =$$

 $\begin{bmatrix}
 1 & 0 \\
 1 & 1 \\
 1 & 0
 \end{bmatrix}$

$$\begin{array}{l} \text{Consider } \widehat{x}_{i} = [1 \ 1] \quad \text{in this data set} \longrightarrow \\ p(\widehat{y}_{i} = 0 \ | \ \widehat{x}_{i}) \propto p(\widehat{x}_{i} = 1 \ | \ \widehat{y}_{i} = 0) p(\widehat{x}_{2} = 1 \ | \ \widehat{y}_{i} = 0) p(\widehat{y}_{i} = 0) \\ = (1) \quad (0.25) \quad (0.4) = 0. | \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 0 \\ 0 \\ 1 & 0 \\ 1$$

Avoiding Underflow

• During the prediction, the probability can underflow:

$$p(y_i = c \mid x_i) \propto \prod_{j=1}^{d} [p(x_{ij} \mid y_i = c)] p(y_i = c)$$

 $\rightarrow All \text{ these are } < 1 \text{ so the product gets very small.}$

 Standard fix is to (equivalently) maximize the logarithm of the probability: Rember that log(ab) = log(a) + log(b) so log(Πa_i) = ξ log(a_i)
 Since log is <u>monotonic</u> the 'c' maximizing p(y_i=c|x_i) also maximizes log p(y_i=c|x_i),
 So maximize log(d/(1) [p(x_i) | y_i=c)] p(y_i=c)) = d/(log(p(x_i) | y_i=c)) + log(p(y_i=c))

Back to Decision Trees

• Instead of validation set, you can use CV to select tree depth.

- But you can also use these to decide whether to split:
 - Don't split if validation/CV error doesn't improve.
 - Different parts of the tree will have different depths.
- Or fit deep decision tree and use CV to prune:
 - Remove leaf nodes that don't improve CV error.

• Popular implementations that have these tricks and others.

Cross-Validation Theory

- Does CV give unbiased estimate of test error?
 - Yes!
 - Since each data point is only used once in validation, expected validation error on each data point is test error.
 - But again, if you CV to select among models then it is no longer unbiased.
- What about variance of CV?
 - Hard to characterize.
 - CV variance on 'n' data points is worse than with a validation set of size 'n'.
 - But we believe it is close.

Handling Data Sparsity

- Do we need to store the full bag of words 0/1 variables?
 - No: only need list of non-zero features for each e-mail.

\$	Hi	CPSC	340	Vicodin	Offer		Non-Zeroes
1	1	0	0	1	0		{1,2,5,}
0	0	0	0	1	1	 VS.	{5,6,}
0	1	1	1	0	0		{2,3,4,}
1	1	0	0	0	1		{1,2,6,}

Math/model doesn't change, but more efficient storage.

Less-Naïve Bayes

- The assumption is very strong, and there are "less naïve" versions:
 - Assume independence of all variables except up to 'k' largest 'j' where j < i.
 - E.g., naïve Bayes has k=0 and with k=2 we would have:

$$\approx \rho(y) \rho(x, ly) \rho(x_2 | x_1, y) \rho(x_3 | x_2, x_1, y) \rho(x_4 | x_3, x_2, y) \cdots \rho(x_d | x_{d-2}, x_{d-1}y)$$

- Fewer independence assumptions so more flexible, but hard to estimate for large 'k'.
- Another practical variation is "tree-augmented" naïve Bayes.

Gaussian Discriminant Analysis

- Classifiers based on Bayes rule are called generative classifier:
 - They often work well when you have tons of features.
 - But they need to know $p(x_i | y_i)$, probability of features given the class.
 - How to "generate" features, based on the class label.
- To fit generative models, usually make BIG assumptions:
 - Naïve Bayes (NB) for discrete x_i:
 - Assume that each variables in x_i is independent of the others in x_i given y_i.
 - Gaussian discriminant analysis (GDA) for continuous x_i.
 - Assume that $p(x_i | y_i)$ follows a multivariate normal distribution.
 - If all classes have same covariance, it's called "linear discriminant analysis".

Computing p(x_i) under naïve Bayes

- Generative models don't need p(x_i) to make decisions.
- However, it's easy to calculate under the naïve Bayes assumption: $p(x_i) = \sum_{i=1}^{k} p(x_{ij}y = c)$ (marginalization rule) $= \sum_{i=1}^{n} p(x_i | y = c) p(y = c) (product rule)$ $= \sum_{c=1}^{K} \left[\prod_{j=1}^{d} p(x_{ij} | y = c) \right] p(y=c) \quad (naive Bayes assumption)$ These are the quantilies we compute during training