CPSC 340: Machine Learning and Data Mining

More Fundamentals + Probabilistic Classification

Term2, 2021

Admin

- Assignment 1 is due tonight: you should be almost done.
  - You can use 1 late day to submit Thursday, 2 for Friday.
  - Solutions will go up on Monday.

Last Time: Training, Testing, and Validation

- Training step:

  Input: set of 'n' training examples x_i with labels y_i

  Output: a model that maps from arbitrary x_i to a $\hat{y}_i$

- Prediction step:

  Input: set of 't' testing examples $\tilde{x}_i$ and a model.

  Output: predictions $\hat{y}_i$ for the testing examples.

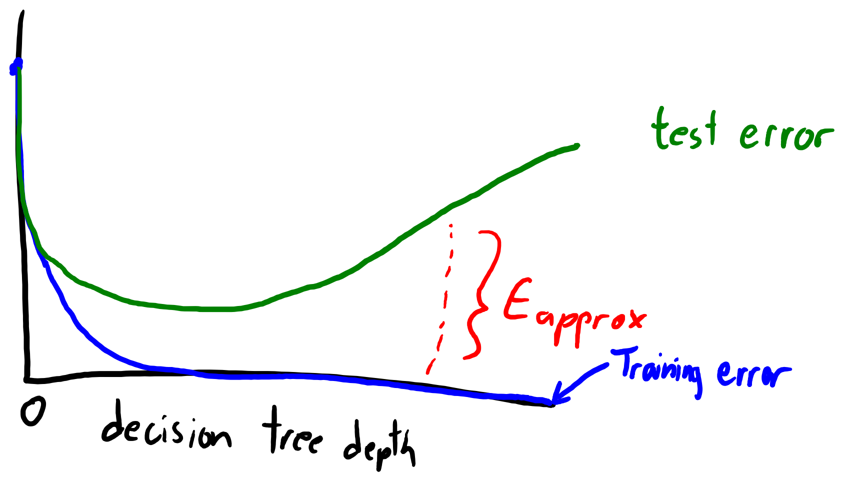
- What we are interested in is the test error:
  - Error made by prediction step on new data.

Last Time: Fundamental Trade-Off

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

$$\underbrace{E_{test}}_{\text{"test error"}} = \underbrace{E_{approx}}_{\text{"approximation error"}} + \underbrace{E_{train}}_{\text{"training error"}}$$

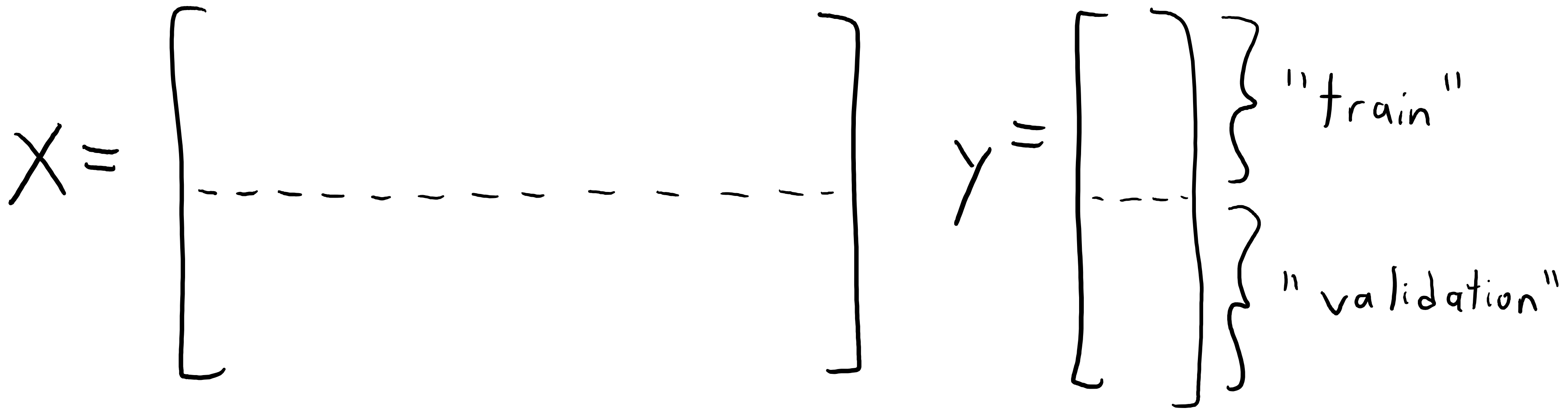
  - Where $E_{approx} = (E_{test} - E_{train})$.



- E_{train} goes down as model gets complicated:
  - Training error goes down as a decision tree gets deeper.
- But E_{approx} goes up as model gets complicated:
  - Training error becomes a worse approximation of test error.

Last Time: Validation Error

- 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.
    - We typically choose "hyper-parameters" like depth to minimize the validation error.

Overfitting to the Validation Set?

- Validation error usually has lower optimization bias than training error.
  - Might optimize over 20 values of “depth”, instead of millions+ of possible trees.

- But we can still overfit to the validation error (common in practice):
  - Validation error is only an unbiased approximation if you use it once.
  - Once you start optimizing it, you start to overfit to the validation set.

- This is most important when the validation set is “small”:
  - The optimization bias decreases as the number of validation examples increases.

- Remember, our goal is still to do well on the test set (new data), not the validation set (where we already know the labels).

Should you trust them?

- 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.

Should you trust them?

- 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 (THE TEST DATA CANNOT INFLUENCE THE TRAINING PHASE IN ANY WAY.).

Should you trust them?

- 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.

Should you trust them?

- 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.
  - 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.

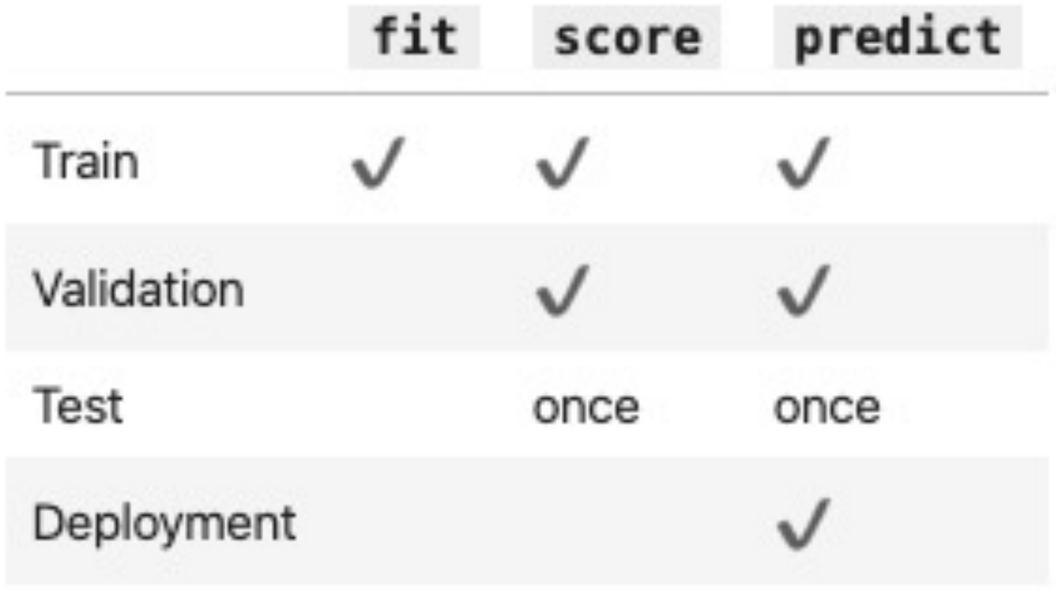
Should you trust them?

- 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.

Train/Validation/Test Terminology

- Training set: used (a lot) to set parameters.
- Validation set: used (a few times) to set hyper-parameters.
- Testing set: used (once) to evaluate final performance.
- Deployment (real-world): what you really care about.



	`fit`	`score`	`predict`
Train	✓	✓	✓
Validation		✓	✓
Test		once	once
Deployment			✓

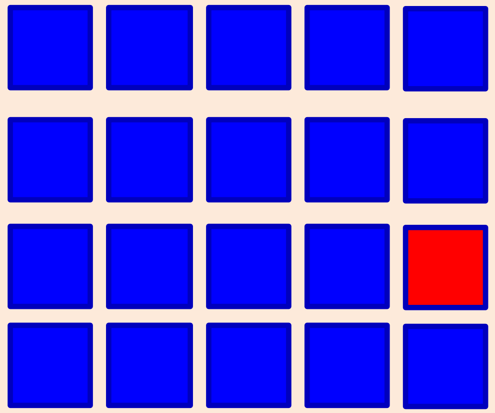
Validation Error and Optimization Bias

- 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.
- And optimization bias shrinks as you grow size of validation set.

bonus!

Aside: Optimization Bias leads to Publication Bias

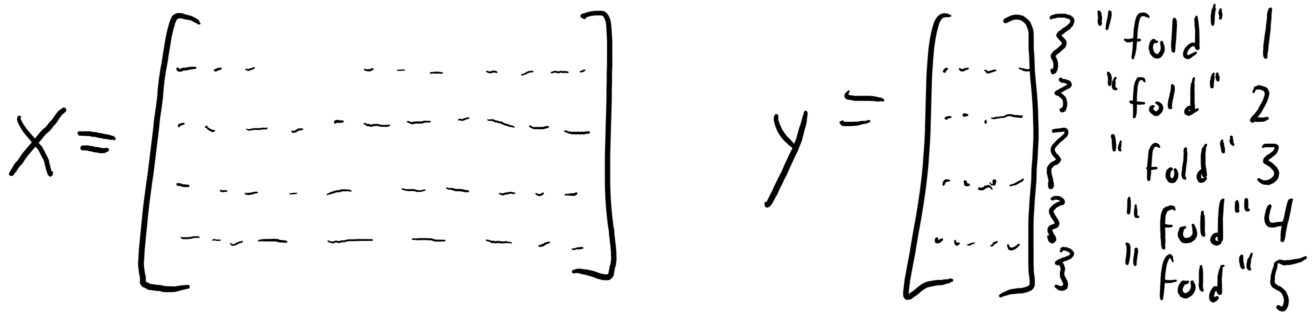
- Suppose that 20 researchers perform the exact same experiment:



- They each test whether their effect is “significant” ($p < 0.05$).
  - 19/20 find that it is not significant.
  - But the 1 group finding it’s significant publishes a paper about the effect.
- This is again optimization bias, contributing to publication bias.
  - A contributing factor to many reported effects being wrong.

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.

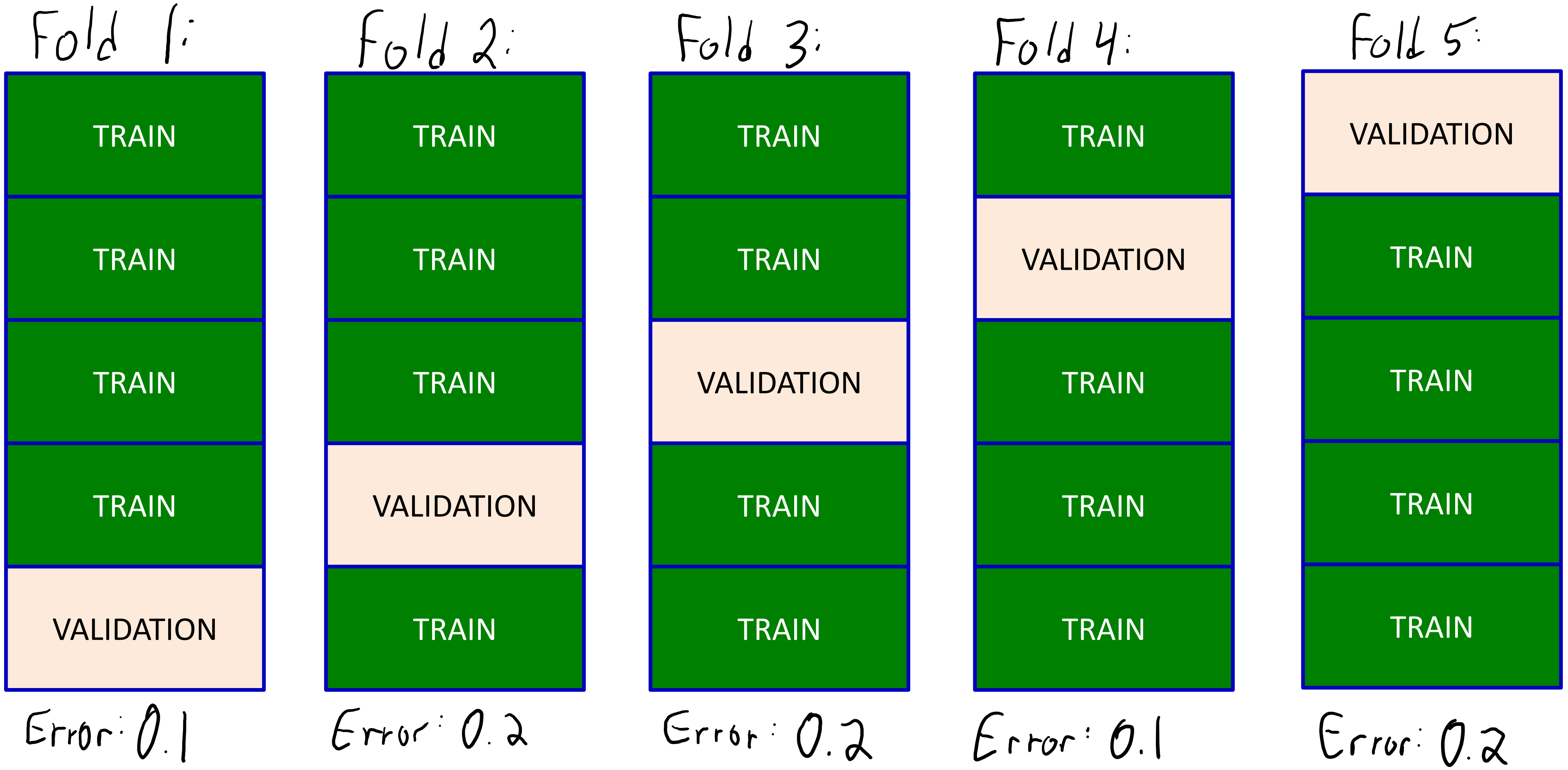


1. Train on folds {1, 2, 3, 4}, compute error on fold 5.
2. Train on folds {1, 2, 3, 5}, compute error on fold 4.
3. Train on folds {1, 2, 4, 5}, compute error on fold 3.

⋮

6. Take $\underbrace{\text{average}}$ of the 5 errors as approximation of test error

Cross-Validation (CV)



CV error estimate for this hyper-parameter: mean(errors) = 0.16

Cross-Validation Pseudo-Code

To choose depth

```
for depth in 1:20
    compute cross-validation score
return depth with highest score
```

To compute 5-fold cross-validation score:

```
for fold in 1:5
    train 80% that doesn't include fold
    test on fold
return average test error
```

Notes:

- This fits 100 models! (20 depths times 5 folds)
- We get one (average) score for each of the 20 depths.
- Use this score to pick depth

Cross-Validation (CV)

- You can take this idea further ("k-fold cross-validation"):
  - 10-fold cross-validation: train on 90% of data and validate on 10%.
    - Repeat 10 times and average (test on fold 1, then fold 2,…, then fold 10),
  - Leave-one-out cross-validation: train on all but one training example.
    - Repeat n times and average.
- Mean score 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.

(pause)

The "Best" Machine Learning Model

- Decision trees are not always most accurate on test error.
- What is the "best" machine learning model?
- Usual measure of performance is the generalization error:
  - Average error for a random new (x, y) from the (hypothetical) data distribution.
  - "How well we expect to do on a *completely fresh* test set."
- No free lunch theorem (proof in bonus slides):
  - 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."

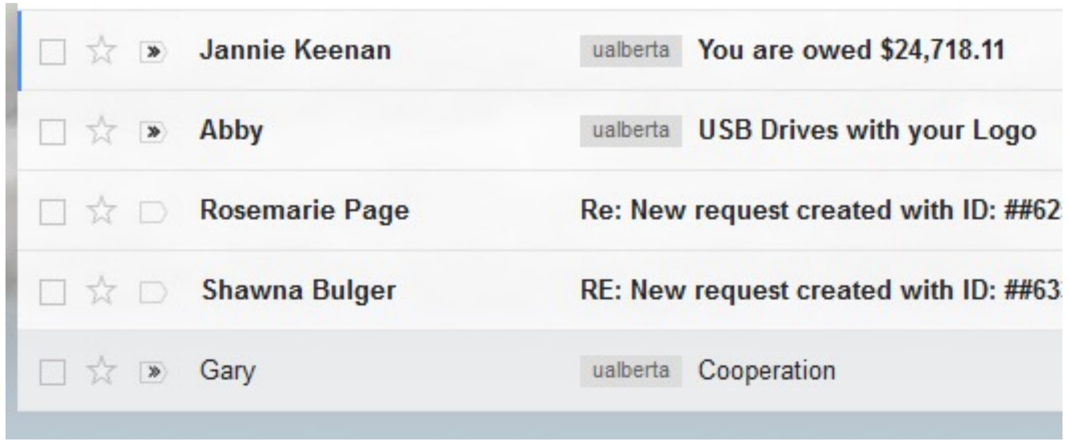
The “Best” Machine Learning Model

- 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.

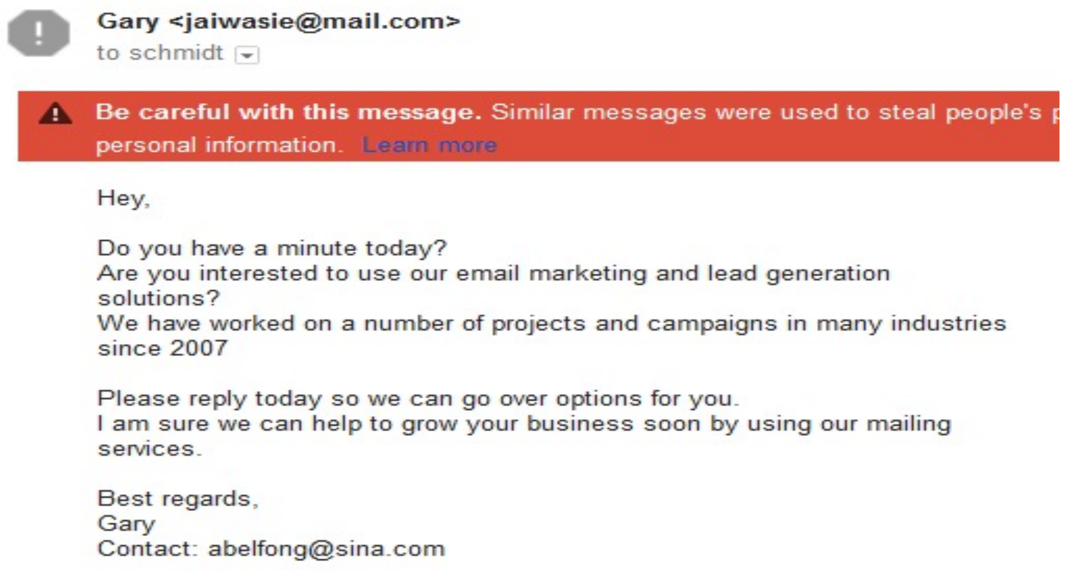
- Caveat of no free lunch (NFL) theorem:
  - The world is very structured.
    - But proof of the no-free-lunch theorem assumes any map from x_i to y_i is equally likely.
  - Some datasets are more likely than others.
  - Model A really could be better than model B on every real dataset in practice.
- 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.



Jannie Keenan	ualberta	You are owed $24,718.11
Abby	ualberta	USB Drives with your Logo
Rosemarie Page		Re: New request created with ID: ##62
Shawna Bulger		RE: New request created with ID: ##63
Gary	ualberta	Cooperation



Gary <jaiwasie@mail.com>
to schmidt

Be careful with this message. Similar messages were used to steal people's p
personal information. Learn more

Hey,

Do you have a minute today?
Are you interested to use our email marketing and lead generation solutions?
We have worked on a number of projects and campaigns in many industries since 2007

Please reply today so we can go over options for you.
I am sure we can help to grow your business soon by using our mailing services.

Best regards,
Gary
Contact: abelfong@sina.com

- 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.

bonus!

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>.

Review of Supervised Learning Notation

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

$X =$

\$	Hi	CPSC	340	Vicodin	Offer	…
1	1	0	0	1	0	…
0	0	0	0	1	1	…
0	1	1	1	0	0	…
…	…	…	…	…	…	…

$\rightarrow x_{26}$

$\rightarrow x_3$

$y =$

Spam?
1
1
0
…

$\rightarrow y_3$

- X is matrix of all features, y is vector of all labels.
  - We use y_i for the label of example 'i' (element 'i' of 'y').
  - We use x_{ij} for feature 'j' of example 'i'.
  - We use x_i as the list of features of example 'i' (row 'i' of 'X').
    - So in the above x_3 = [0 1 1 1 0 0 …].
    - In practice, only store list of non-zero features for each x_i (small memory requirement).

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.
  - Recently shown to improve on state of the art for CRISPR "gene editing" (link).

- Probabilistic classifiers model the conditional probability, $p(y_i \mid x_i)$.
  - "If a message has words x_i, what is probability that message is spam?"

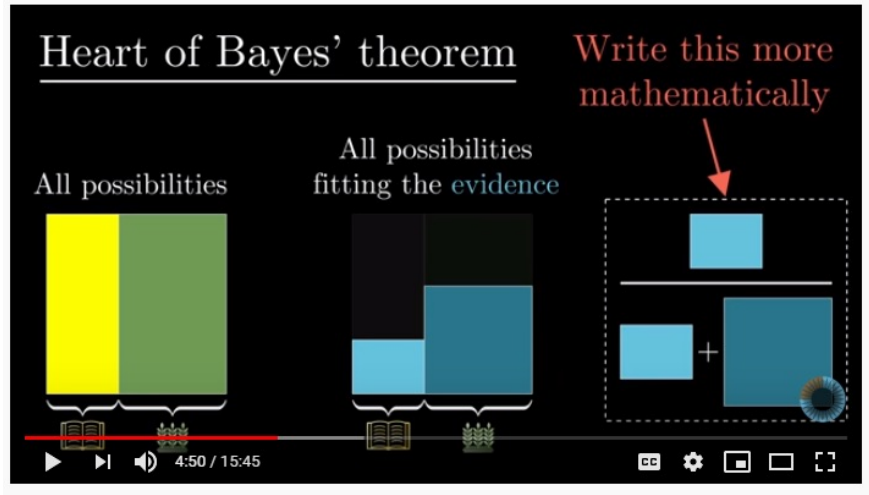
- Classify it as spam if probability of spam is higher than not spam:
  - If $p(y_i = \text{"spam"} \mid x_i) > p(y_i = \text{"not spam"} \mid x_i)$
    - return "spam".
  - Else
    - return "not spam".

Spam Filtering with Bayes Rule

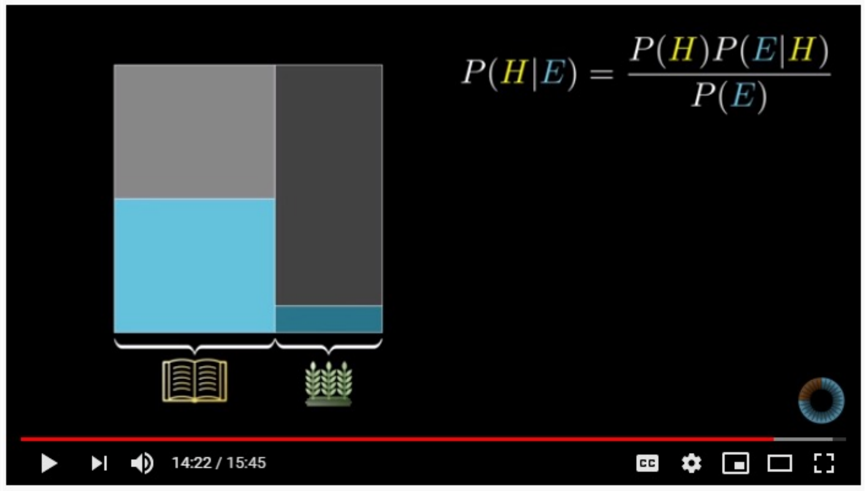
- To model conditional probability, naïve Bayes uses Bayes rule:

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- Nice video giving visual intuition for Bayes rule here:



Heart of Bayes' theorem
Write this more mathematically
All possibilities
All possibilities fitting the evidence
4:50 / 15:45



Spam Filtering with Bayes Rule

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

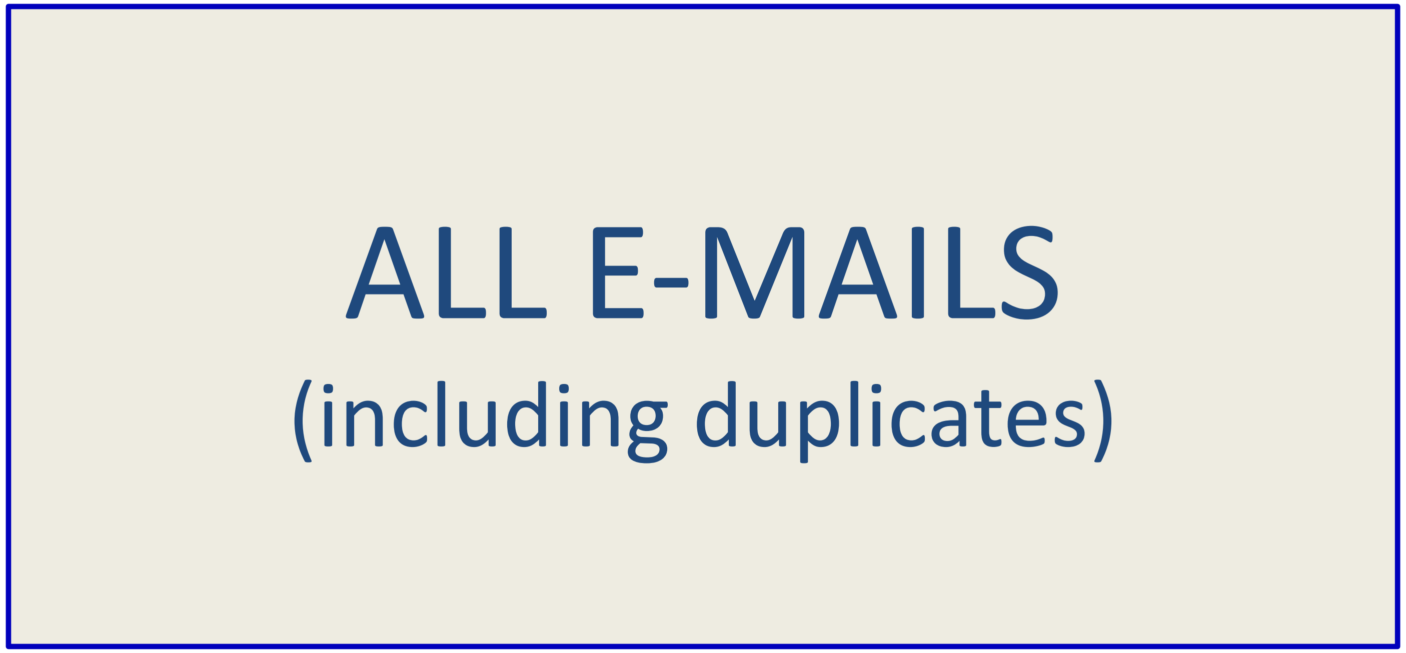
$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- On the right we have three terms:
  - Marginal probability $p(y_i)$ that an e-mail is spam.
  - Marginal probability $p(x_i)$ that an e-mail has the set of words x_i.
  - Conditional probability $p(x_i \mid y_i)$ that a spam e-mail has the words x_i.
    - And the same for non-spam e-mails.

Spam Filtering with Bayes Rule

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

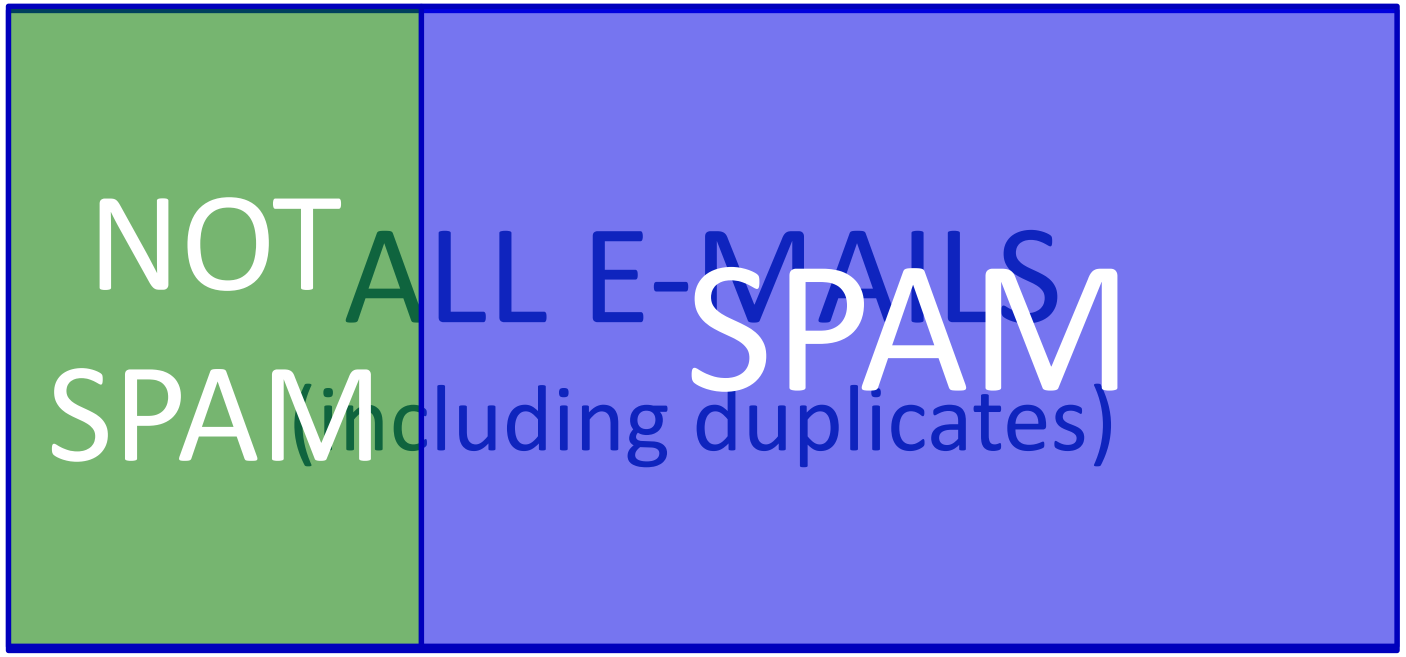
- What do these terms mean?



Spam Filtering with Bayes Rule

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- 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.



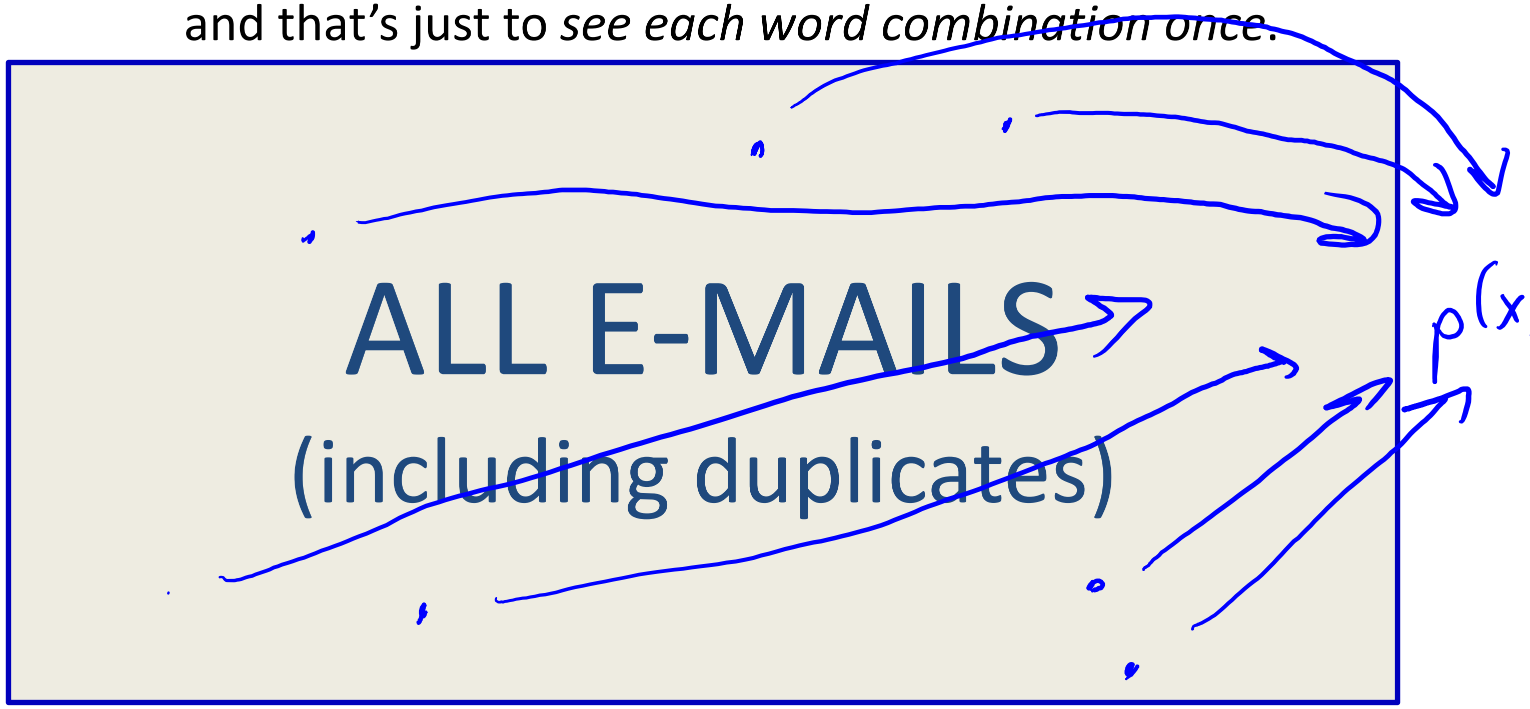
$$p(y_i = \text{"spam"}) = \frac{\#\text{ spam messages}}{\#\text{ total messages}}$$

This is an "estimate" of the true probability. In particular, this formula is a "maximum likelihood estimate" (MLE). We will cover likelihoods and MLEs later in the course.

Spam Filtering with Bayes Rule

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- $p(x_i)$ is probability that a random e-mail has features x_i:
  - Hard to approximate: with 'd' words we need to collect 2^d "coupons", and that's just to *see each word combination once*.



$$p(x_i) = \frac{\#\text{ e-mails with features } x_i}{\#\text{ e-mails total}}$$

Spam Filtering with Bayes Rule

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- $p(x_i)$ is probability that a random e-mail has features x_i:
  - Hard to approximate: with 'd' words we need to collect 2^d "coupons", but it turns out we can ignore it:

Naive Bayes returns "spam" if $p(y_i = \text{"spam"} \mid x_i) > p(y_i = \text{"not spam"} \mid x_i)$.

By Bayes rule this means $\frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)} > \frac{p(x_i \mid y_i = \text{"not spam"})\, p(y_i = \text{"not spam"})}{p(x_i)}$

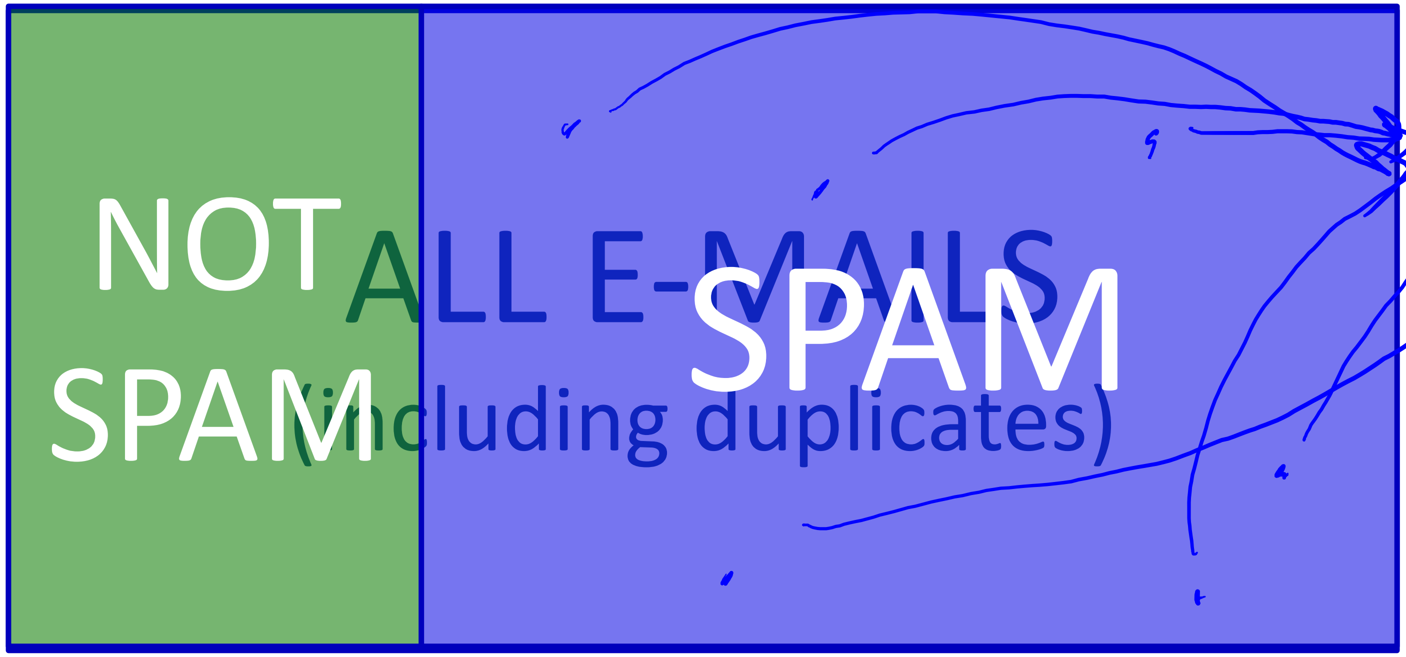
Multiply both sides by $p(x_i)$:

$$p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"}) > p(x_i \mid y_i = \text{"not spam"})\, p(y_i = \text{"not spam"})$$

Spam Filtering with Bayes Rule

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- $p(x_i \mid y_i = \text{"spam"})$ is probability that spam has features x_i.



$$p(x_i \mid y_i = \text{"spam"}) = \frac{\#\ \underline{\text{spam}}\ \text{messages with}\ \underline{\text{features}}\ x_i}{\#\ \text{spam messages}}$$

- Also hard to approximate.
  - And we need it.

Naïve Bayes

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

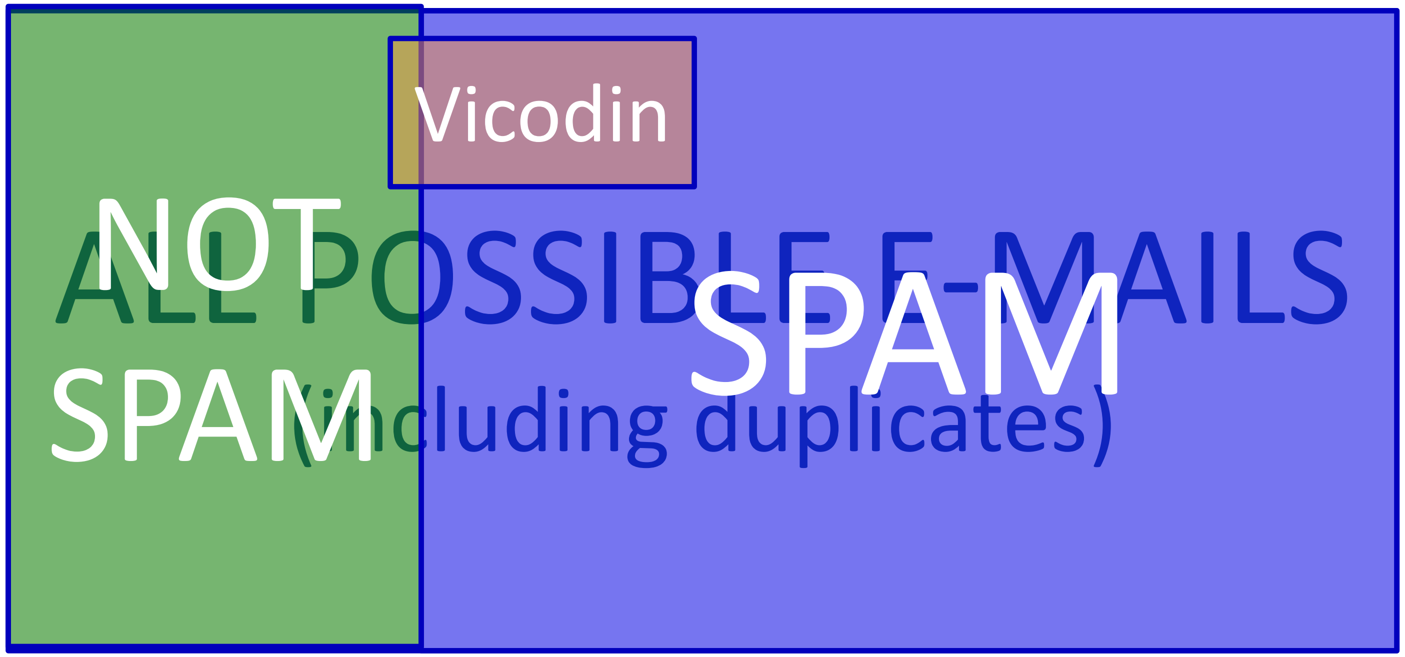
$$\underbrace{p(\text{hello}=1, \text{vicodin}=0, 340=1 \mid \text{spam})}_{\text{HARD}} \approx \underbrace{p(\text{hello}=1 \mid \text{spam})}_{\text{easy}} \underbrace{p(\text{vicodin}=0 \mid \text{spam})}_{\text{easy}} \underbrace{p(340=1 \mid \text{spam})}_{\text{easy}}$$

- 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 "340".
  - *Definitely not true*, but sometimes a good approximation.

- And now we only need easy quantities like p("vicodin" = 0| y_i = "spam").

Naïve Bayes

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



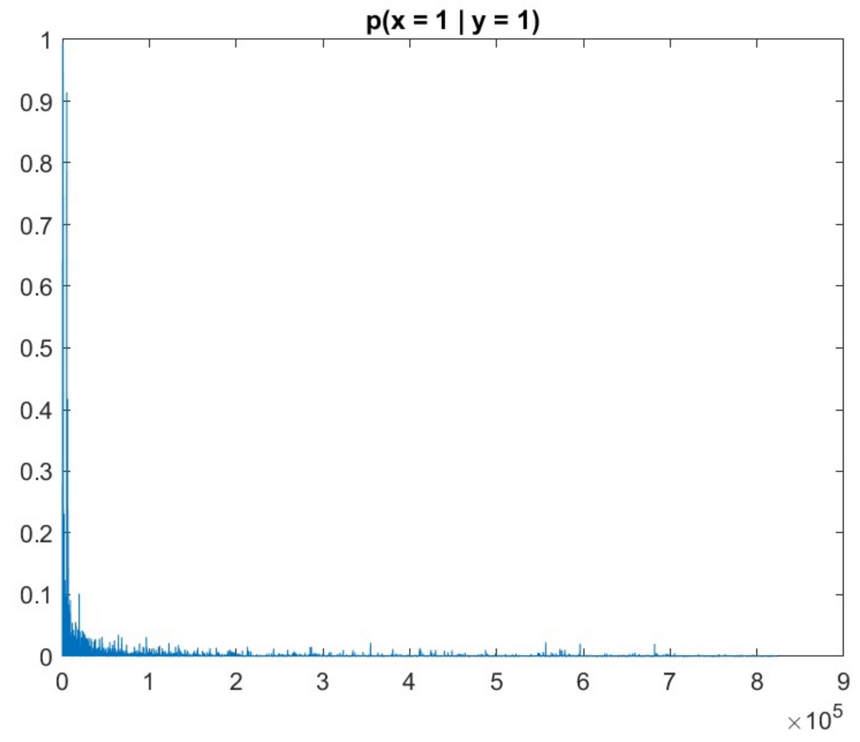
- Easy to estimate:

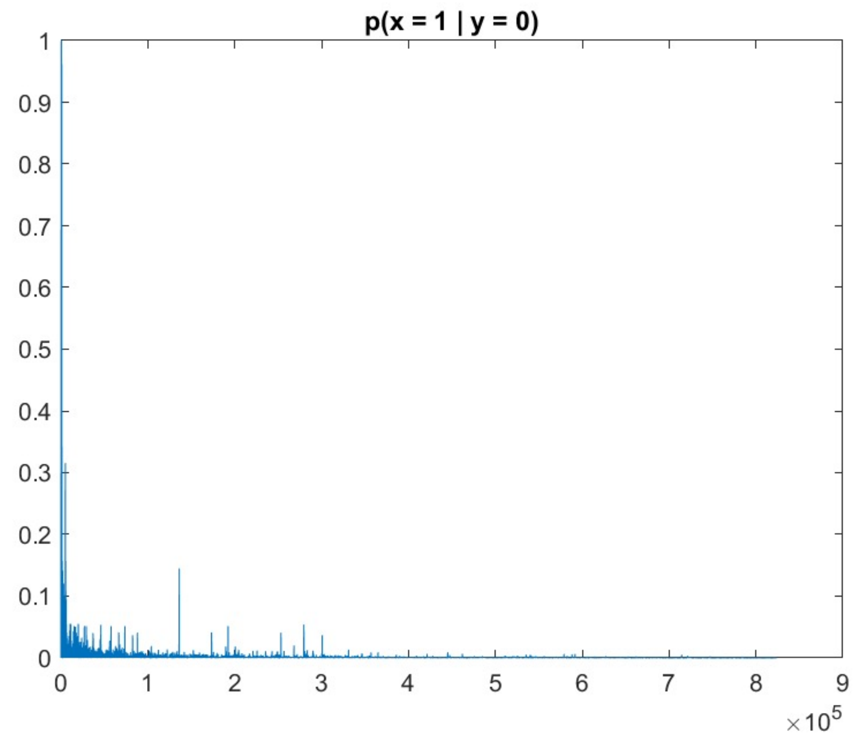
$$p(\text{vicodin}=1 \mid \text{spam}=1) = \frac{\#\text{ spam messages w/ vicodin}}{\#\text{ spam messages}}$$

Again, this is a "maximum likelihood estimate" (MLE). We will cover how to derive this later.

Naïve Bayes

- Comparing p(x | y = c) for “spam” and “not spam”:





- Even though independence is not true,
  these values may be enough to distinguish the classes.

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 $p(y_i \mid x_i)$.
- 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 ∞.

bonus!

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 [cross-]validation to prune:
  - Remove leaf nodes that don’t improve CV error.

- Popular implementations that have these tricks and others.

bonus!

Random Subsamples

- Instead of splitting into k-folds, consider "random subsample" method:
  - At each "round", choose a random set of size 'm'.
    - Train on all examples except these 'm' examples.
    - Compute validation error on these 'm' examples.

- Advantages:
  - Still an unbiased estimator of error.
  - Number of "rounds" does not need to be related to "n".
- Disadvantage:
  - Examples that are sampled more often get more "weight".

bonus!

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 use 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.

- Does cross-validation remove optimization bias?
  - No, but the bias might be smaller since you have more “test” points.

bonus!

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	…
1	1	0	0	1	0	…
0	0	0	0	1	1	…
0	1	1	1	0	0	…
1	1	0	0	0	1	…

vs.

Non-Zeroes
{1,2,5,…}
{5,6,…}
{2,3,4,…}
{1,2,6,…}

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

bonus!

Generalization Error

- Usual measure of performance is the generalization error:
  - Average error for a random new (x, y) from the (hypothetical) data distribution.
  - "How well we expect to do on a *completely fresh* test set."
- Test error vs. generalization error when labels are deterministic:

$$E_{test} = \mathbb{E}[|\hat{y}^i - \tilde{y}^i|] \qquad E_{generalize} = \frac{1}{t}\sum_{\tilde{x}^i \notin \{\text{train set}\}} |\hat{y}_i - \tilde{y}_i|$$

Labels are deterministic, but we still take expectation over data distribution

number of x^i values not in training set.

average error over unseen x^i values.

bonus!

“Best” and the “Good” Machine Learning Models

- Question 1: what is the “best” machine learning model?
  - The model that gets lower generalization error than all other models.
- Question 2: which models always do better than random guessing?
  - Models with lower generalization error than “predict 0” for all problems.

- 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.

bonus!

No Free Lunch Theorem

- Let's show the "no free lunch" theorem in a simple setting:
  - The x^i and y^i are binary, and y^i being a deterministic function of x^i.
- With 'd' features, each "learning problem" is a map from $\{0,1\}^d$ -> $\{0,1\}$.
  - Assigning a binary label to each of the 2^d feature combinations.

Feature 1	Feature 2	Feature 3
0	0	0
0	0	1
0	1	0
…	…	…

y (map 1)	y (map 2)	y (map 3)	…
0	1	0	…
0	0	1	…
0	0	0	…
…	…	…	…

- Let's pick one of these 'y' vectors ("maps" or "learning problems") and:
  - Generate a set training set of 'n' IID samples.
  - Fit model A (convolutional neural network) and model B (naïve Bayes).

bonus!

No Free Lunch Theorem

- Define the "unseen" examples as the $(2^d - n)$ not seen in training.
  - Assuming no repetitions of x^i values, and $n < 2^d$.
  - Generalization error is the average error on these "unseen" examples.
- Suppose that model A got 1% error and model B got 60% error.
  - We want to show model B beats model A on another "learning problem".

- Among our set of "learning problems" find the one where:
  - The labels y^i agree on all training examples.
  - The labels y^i disagree on all "unseen" examples.
- On this other "learning problem":
  - Model A gets 99% error and model B gets 40% error.

bonus!

Proof of No Free Lunch Theorem

- Let’s show the “no free lunch” theorem in a simple setting:
  - The x^i and y^i are binary, and y^i being a deterministic function of x^i.
- With ‘d’ features, each “learning problem” is a map from each of the 2^d feature combinations to 0 or 1: $\{0,1\}^d \rightarrow \{0,1\}$

Feature 1	Feature 2	Feature 3
0	0	0
0	0	1
0	1	0
…	…	…

Map 1	Map 2	Map 3	…
0	1	0	…
0	0	1	…
0	0	0	…
…	…	…	…

- Let’s pick one of these maps (“learning problems”) and:
  - Generate a set training set of ‘n’ IID samples.
  - Fit model A (convolutional neural network) and model B (naïve Bayes).

bonus!

Proof of No Free Lunch Theorem

- Define the "unseen" examples as the $(2^d - n)$ not seen in training.
  - Assuming no repetitions of x^i values, and $n < 2^d$.
  - Generalization error is the average error on these "unseen" examples.
- Suppose that model A got 1% error and model B got 60% error.
  - We want to show model B beats model A on another "learning problem".

- Among our set of "learning problems" find the one where:
  - The labels y^i agree on all training examples.
  - The labels y_i disagree on all "unseen" examples.
- On this other "learning problem":
  - Model A gets 99% error and model B gets 40% error.

bonus!

Proof of No Free Lunch Theorem

- Further, across all “learning problems” with these ‘n’ examples:
  - Average generalization error of **every** model is 50% on unseen examples.
    - It’s right on each unseen example in exactly half the learning problems.
  - With ‘k’ classes, the average error is (k-1)/k (random guessing).

- This is kind of depressing:
  - For general problems, no “machine learning” is better than “predict 0”.

- But the proof also reveals the problem with the NFL theorem:
  - Assumes every “learning problem” is equally likely.
  - World encourages patterns like “similar features implies similar labels”.