CPSC 340:
Machine Learning and Data Mining

Probabilistic Classification

Summer 2021

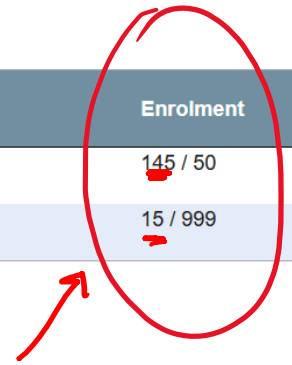
Admin

- Monday:
  - Assignment 1 due
  - Assignment 2 out, due the following Monday
- Next Friday: Assignment 3 out
  - Due the following Friday
  - To make enough time for you to study for midterm
- Midterm will be Tuesday, June 1, 2021
  - Canvas for autograded portion
  - Gradescope for manually graded portion
  - Stay tuned for instructions
- Piazza: partner search post is up.
  - See my recommendations for teamwork.
- Contact us on Piazza if you need help with Gradescope.

Waiting List Situation

You are assigned to the following sections in 2021S:

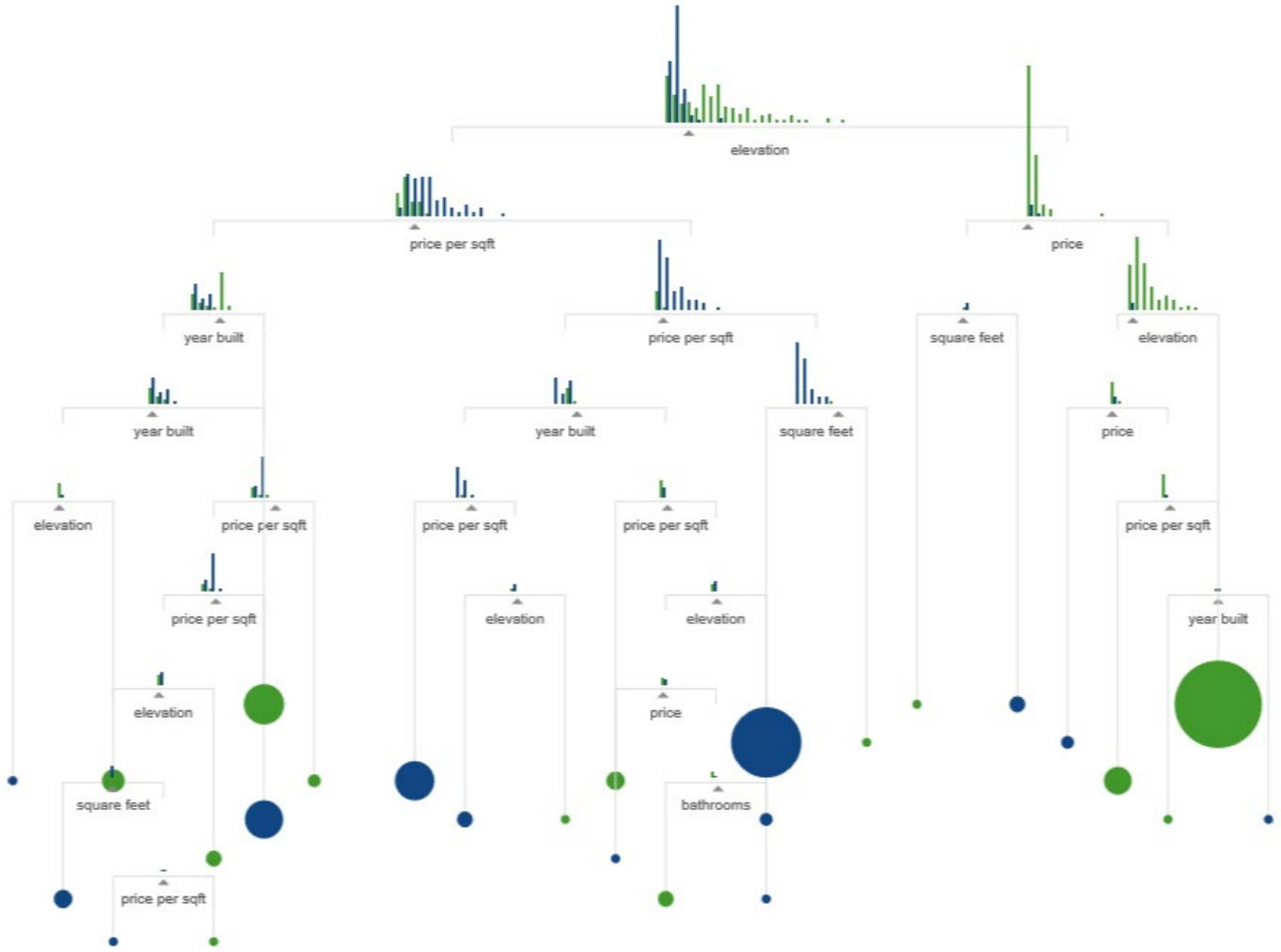
Select All	Course	Term	Starts	Ends	Meetings	Enrolment
☐	CPSC340 - 911	1	2021-05-10	2021-06-17	MonWedFri: 9:30 AM to 12:00 PM	145 / 50
☐	CPSC340 - 9W1	1	2021-05-10	2021-06-17	MonWedFri: 9:30 AM to 12:00 PM	15 / 999



In This Lecture

- More on Optimization Bias (10 minutes)
- Cross-Validation (10 minutes)
- "Best" Machine Learning Model (10 minutes)
- Naïve Bayes (20 minutes)

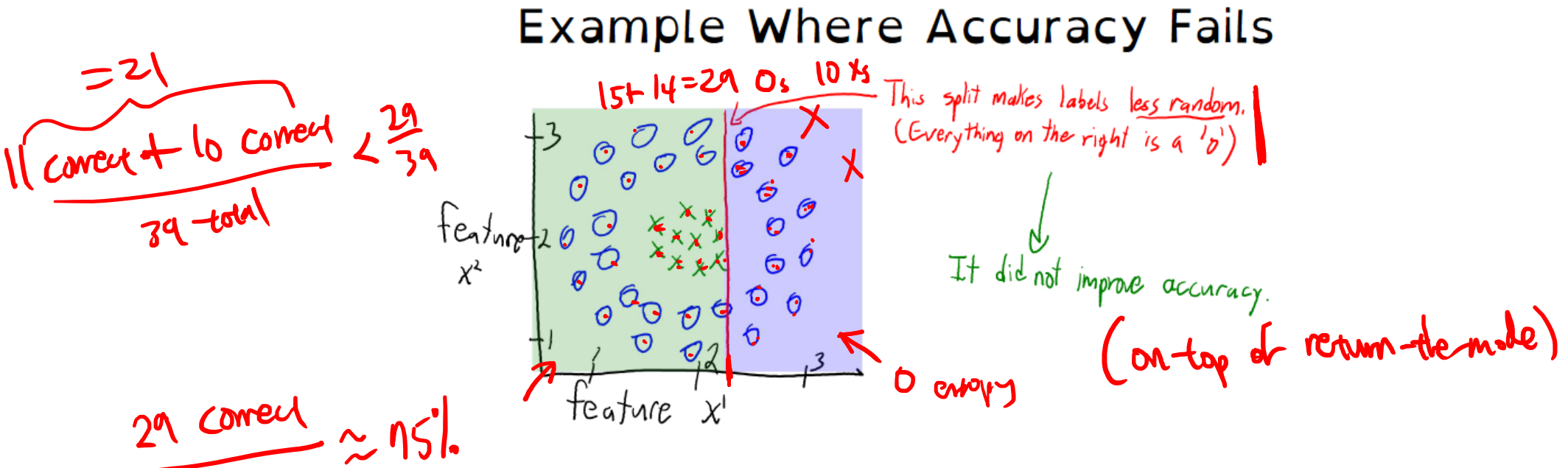
Last Time: Decision Trees



Clarification: Score

- Be careful about how scores are implemented in code.
  - Maximizing accuracy = Minimizing error.
  - We want to (maximize/minimize) information gain
  - Baseline accuracy is accuracy return-the-mode.
  - Baseline information gain is 0.

Clarification: Baseline



- Recall: my baseline is return-the-mode.
- When searching for a decision stump with accuracy score, we should try to beat the baseline, not "accuracy=0"
- Using "accuracy=0" as baseline, you will get a different behaviour.
  - E.g. GRS will actually continue splitting, since we get accuracy > 0 from above split.

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.

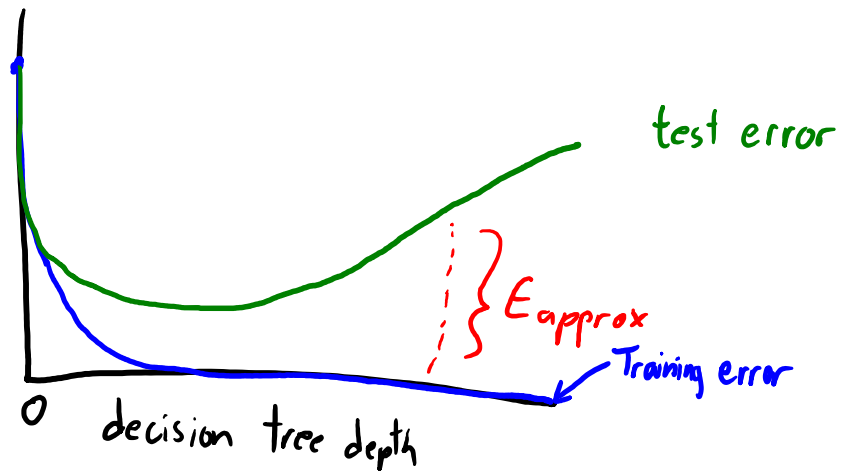
Last Time: Fundamental Trade-Off

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

$$E_{test} = E_{approx} + E_{train}$$

"test error" = "approximation error" + "training error"

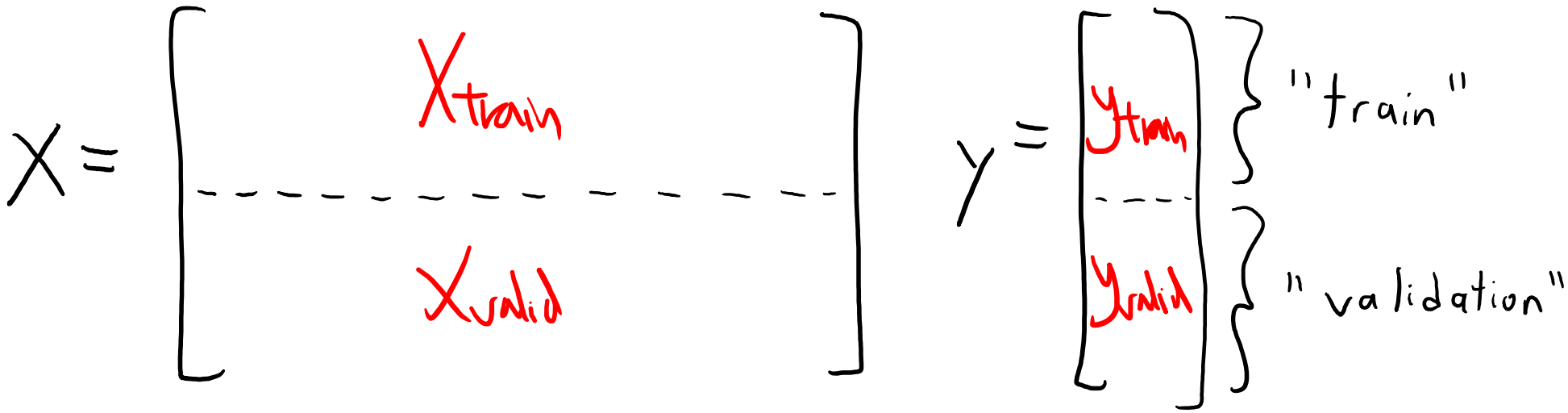
  - Where $E_{approx} = (E_{test} - E_{train})$.



- 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.

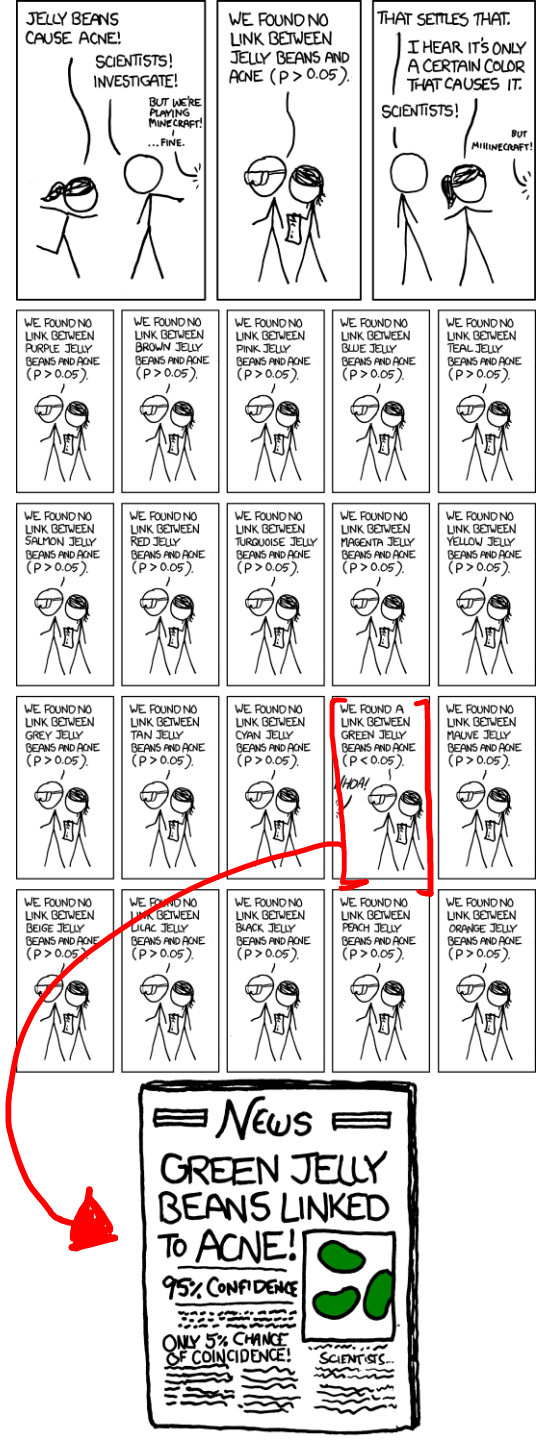
Last Time: Validation Error

- 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.

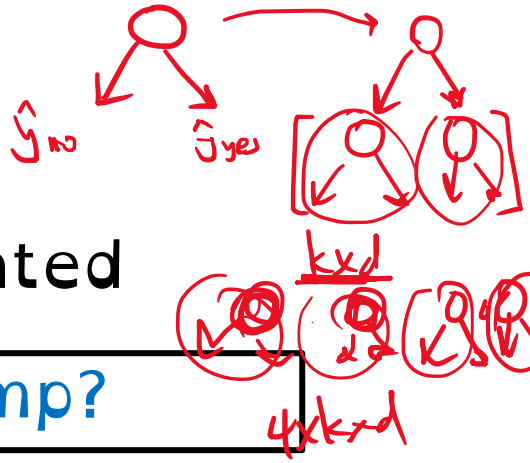
P-value hacking:
One instance of optimization bias
https://xkcd.com/882/



Coming Up Next

MORE ON OPTIMIZATION BIAS

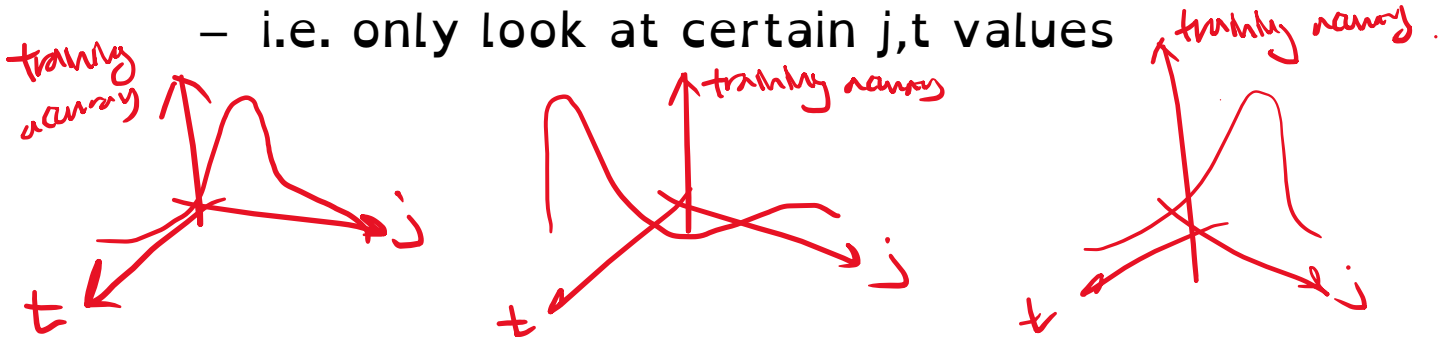
"Search Space"



- Search space := the space of objects that are evaluated

Q: What is the search space for a decision stump?

- We looked at the grid of all possible {j,t} values
- $j \in \{1, 2, \ldots, d\}$, $t \in \{1, 2, \ldots, k\}$
- Search space is a d-by-k grid
  - Enumerating all possible decision stumps
- We evaluated all of the d-by-k grid
  - i.e. we evaluate the training error d*k times
- You could make the search space smaller
  - i.e. only look at certain j,t values



Space of possible decision stumps

"Search Space"

Q: Between training error and validation error, which one has lower optimization bias for decision trees?

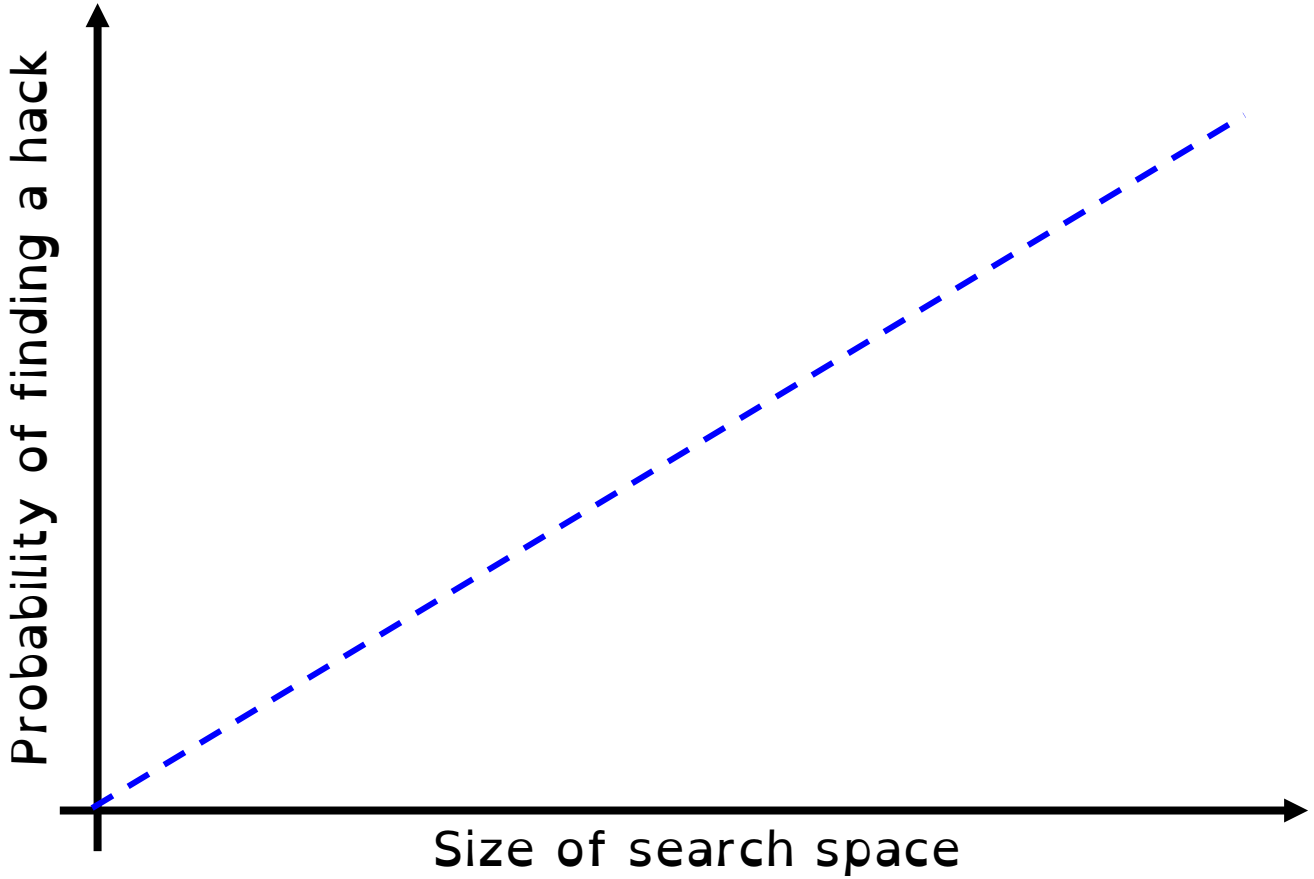
Q: What are the search spaces associated with training error and validation error?

Used to optimize	Used to optimize
parameters	hyper-parameters
Search space for training error:	Search space for validation error:
Space of possible trees	Space of possible depth
	$\in \{1, 2, 3, \cdots, 20\}$

Larger search space => more optimization bias

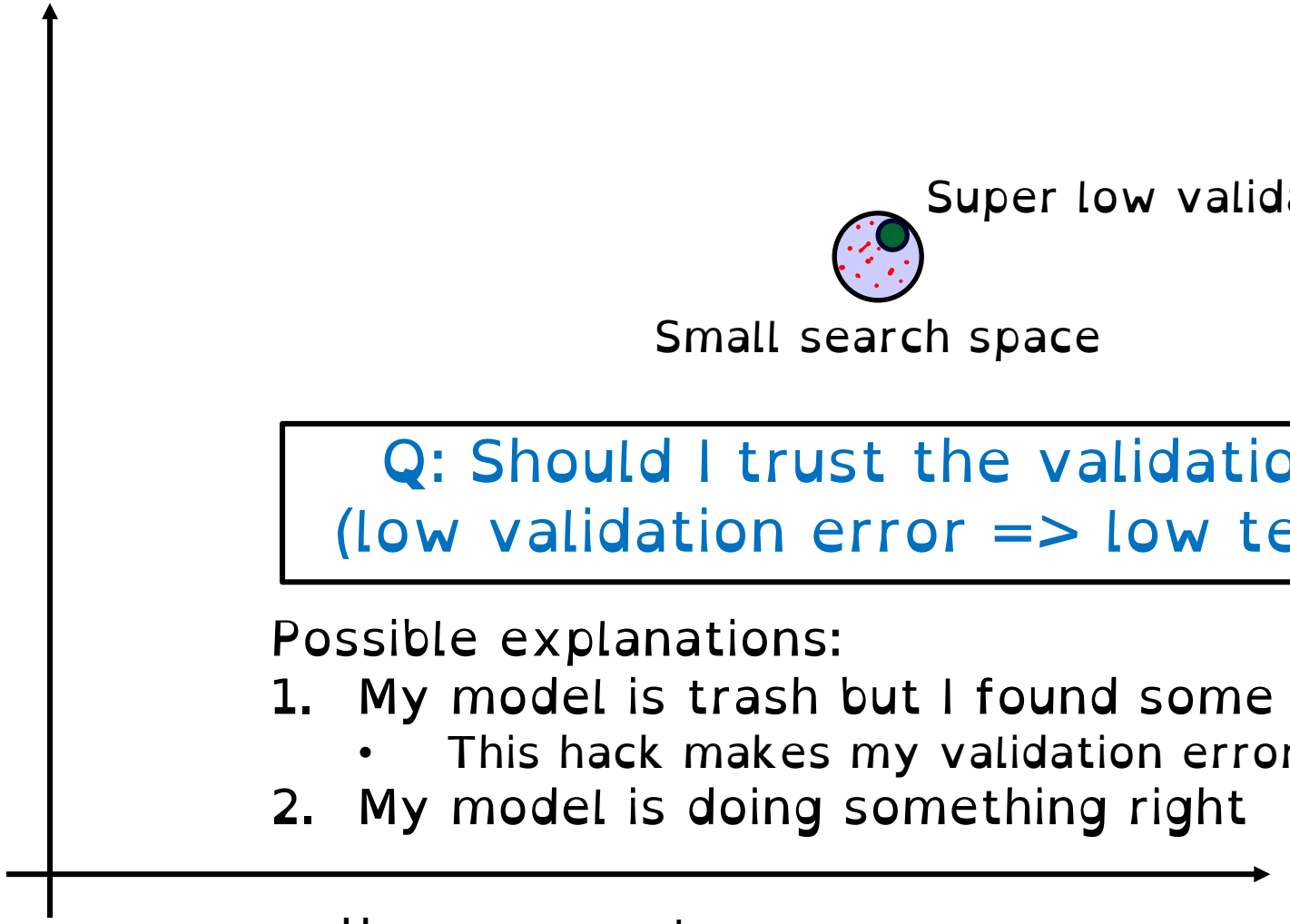
Finding a “Hack” Instead of Learning

- Achieve high score in boat-racing
  - Not by finishing race
  - Circle around infinitely collecting bonus
  - “reward hacking”



https://openai.com/blog/faulty-reward-functions/

Search Space and Optimization Bias

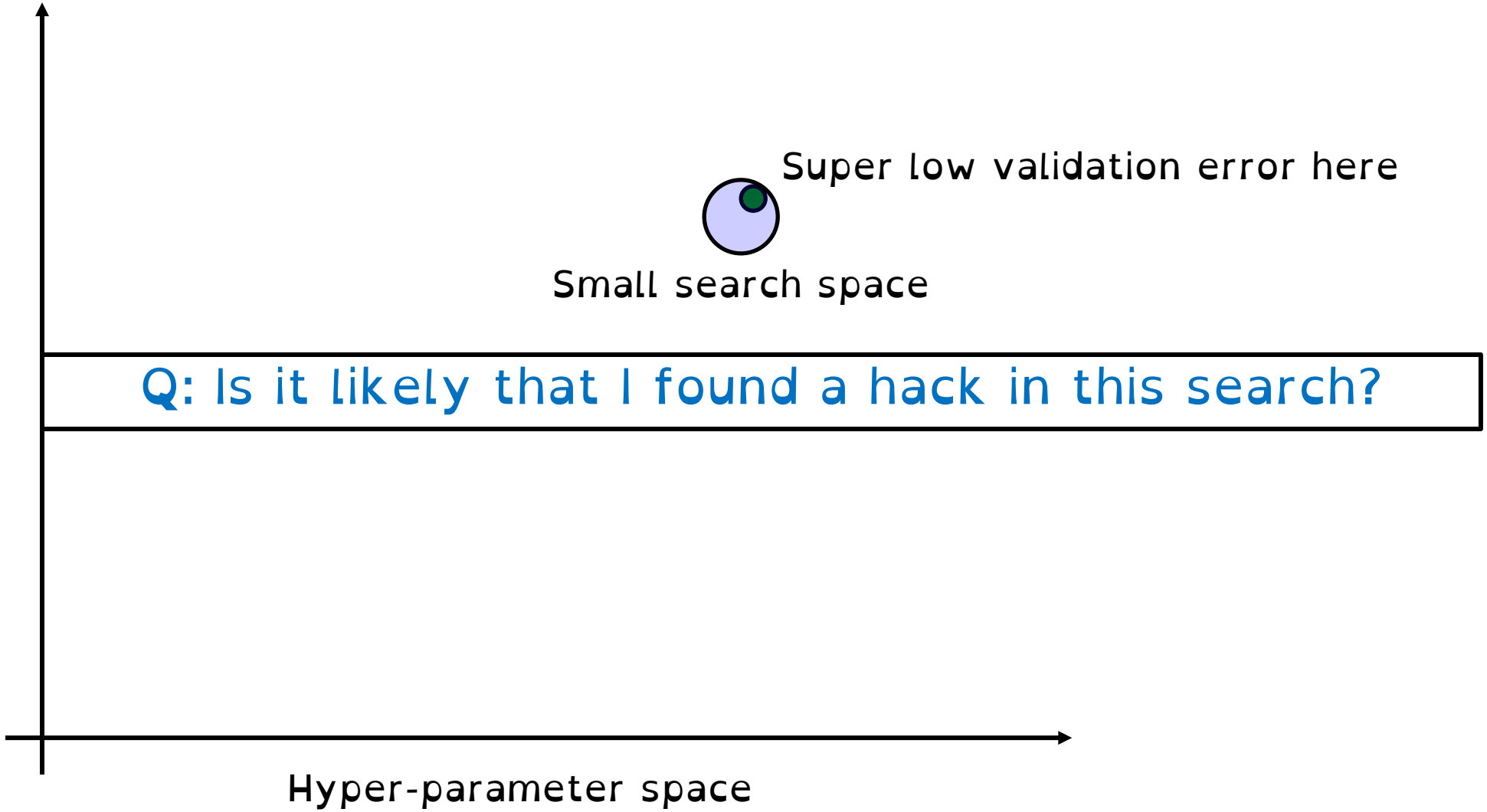


Q: Should I trust the validation error?
(low validation error => low test error?)

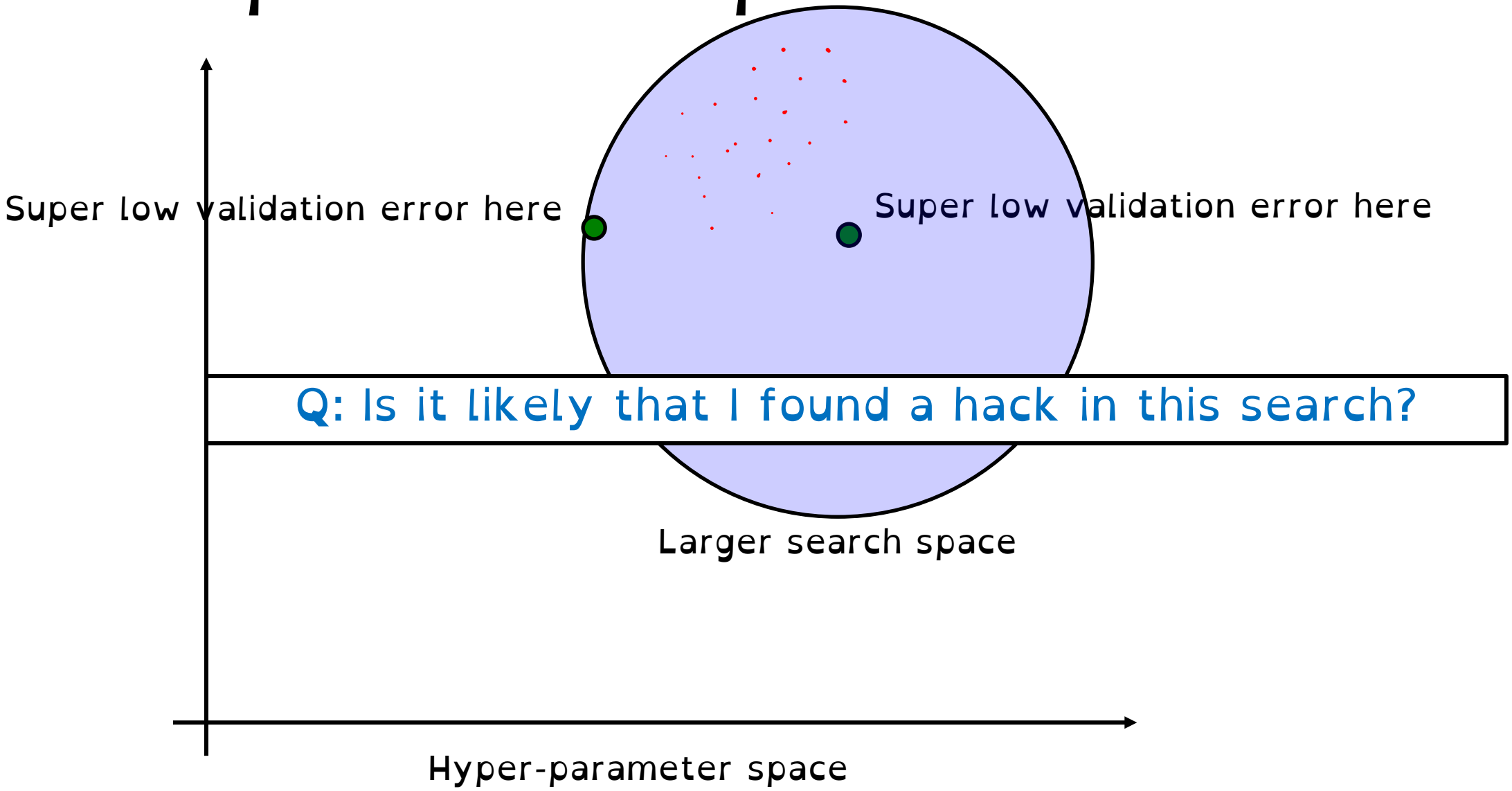
Possible explanations:

1. My model is trash but I found some “hack value”
   - This hack makes my validation error low
2. My model is doing something right

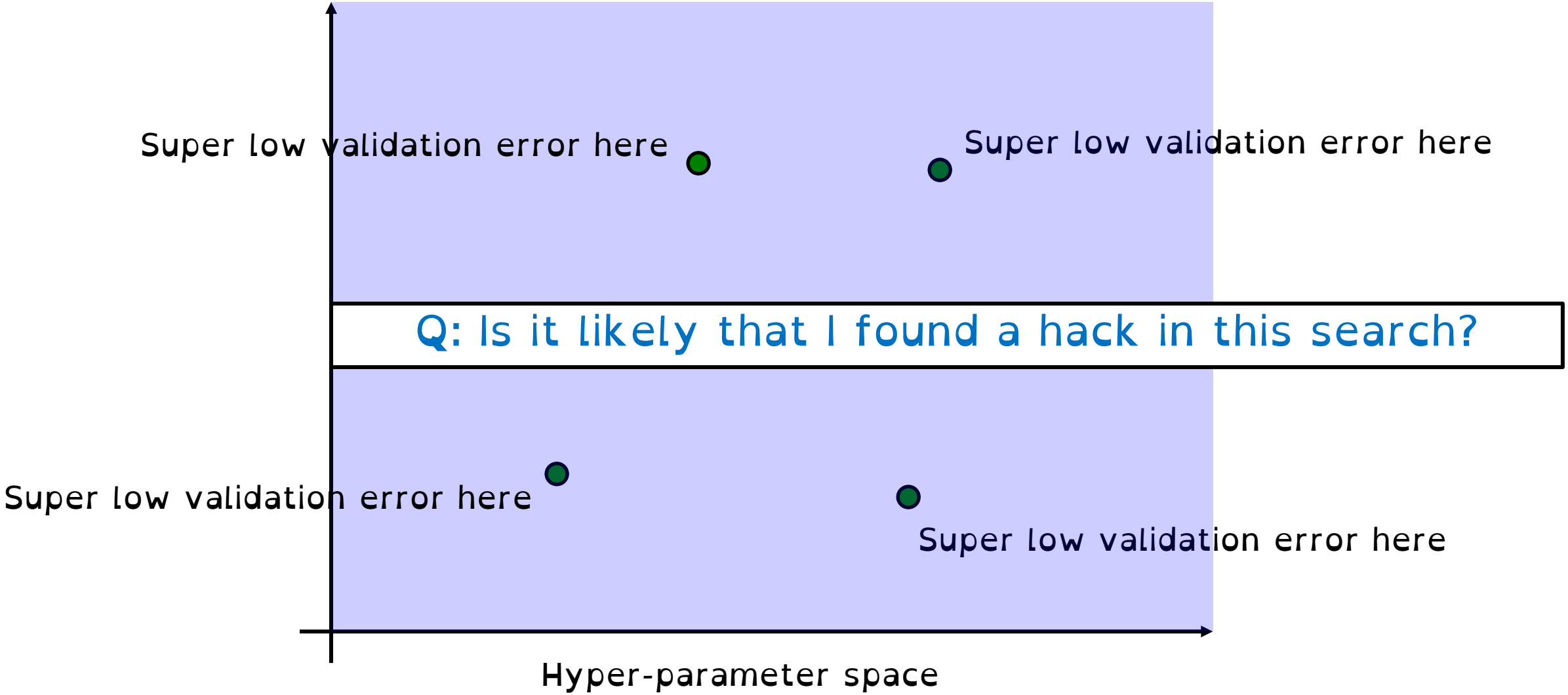
Search Space and Optimization Bias



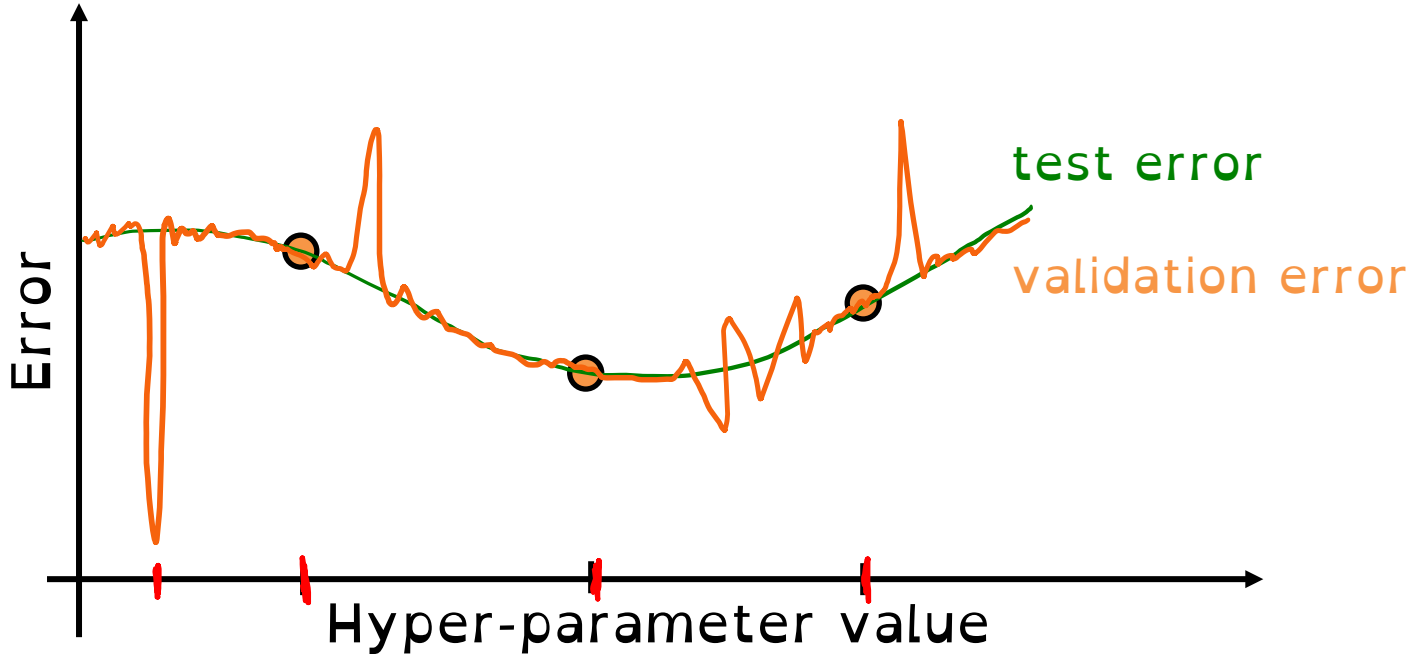
Search Space and Optimization Bias



Search Space and Optimization Bias

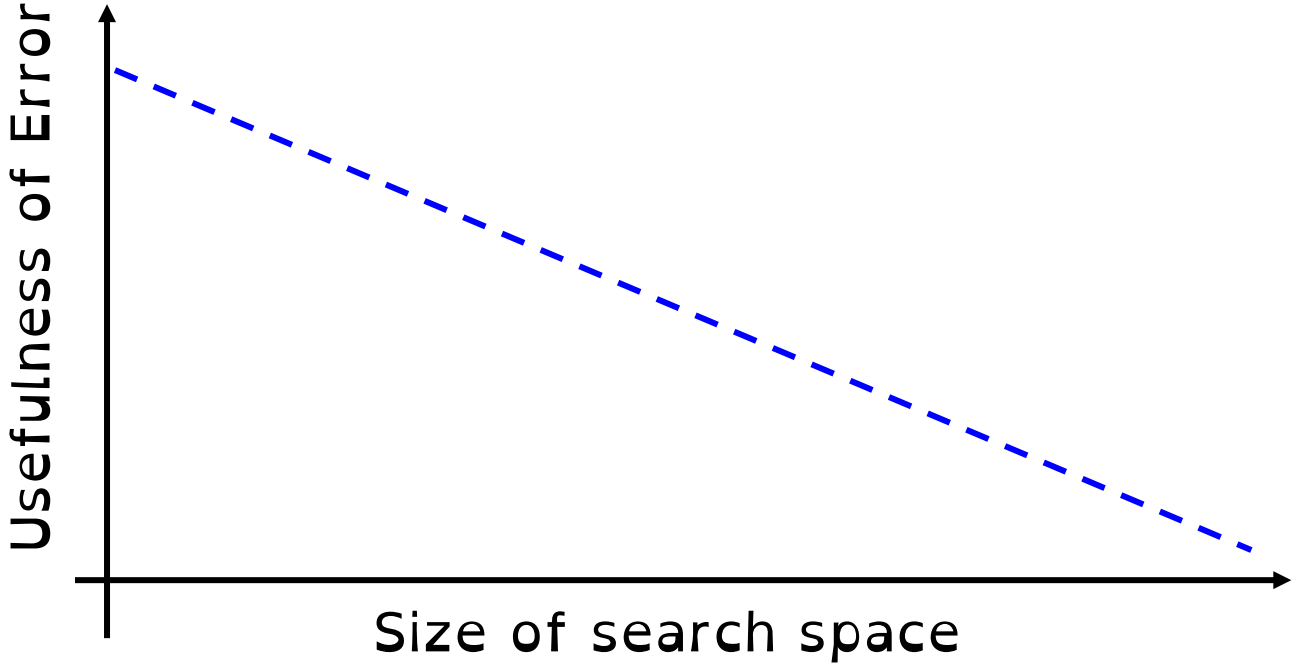


Validation Error Might Do This



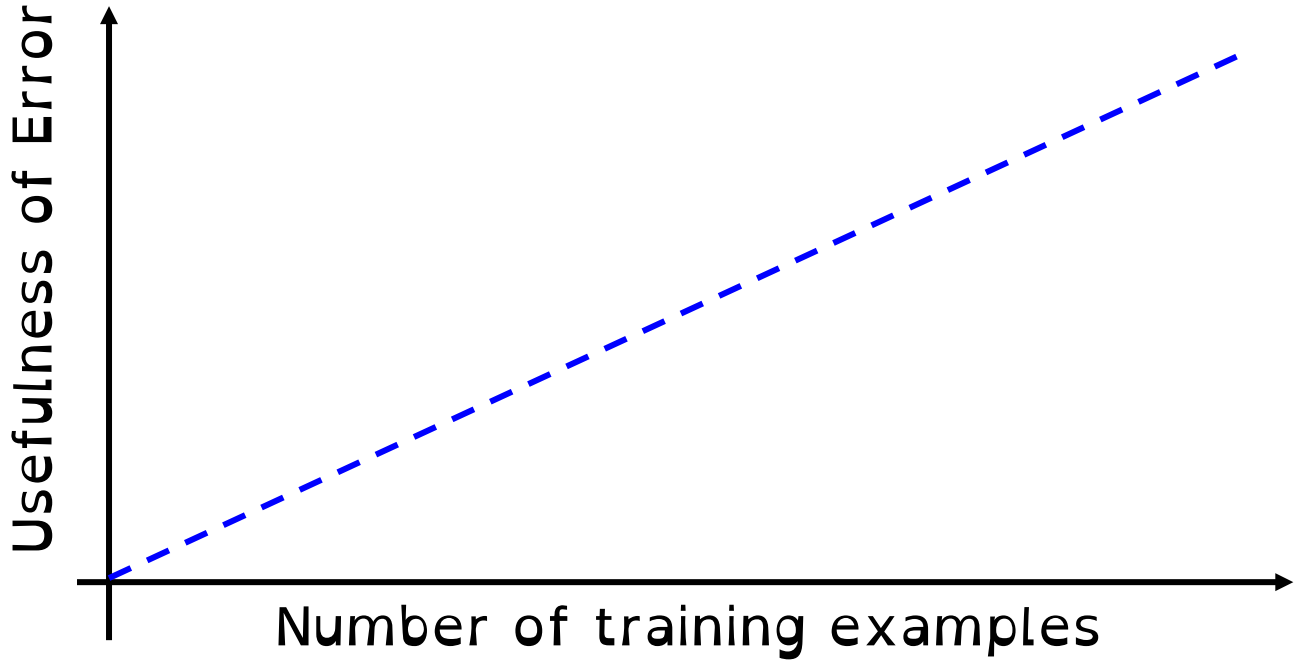
- Noise in the data can make validation error behave strangely in a very fine scale

Is Validation Error Trustworthy?



- Large search space => training error is not trustworthy
- Smaller search space => validation error is more trustworthy
- The more you look validation error, it becomes less trustworthy
- It's best to look the validation error only once
  - In practice, a "small" number of times is good enough

Is Validation Error Trustworthy?



- More training examples => better representation of distribution
  - Under IID, training examples and test examples become more similar
  - Likewise, validation examples and test examples become more similar
- It becomes harder to find a "lucky" case with more training examples

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.

evaluating model with set
. accuracy
. error
. prediction performance.

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

Validation Error and Optimization Bias

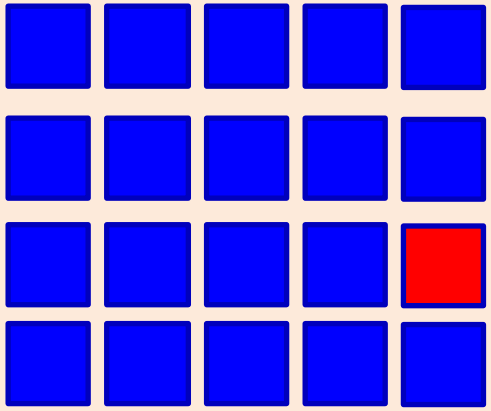
- Optimization bias is small if you only compare a few models:
  - Best decision tree on the training set among depths 1, 2, 3,…, 10.
  - Risk of overfitting to validation set is low if we try 10 things.

- 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.

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.

Coming Up Next

CROSS-VALIDATION

Recall: E_{valid} and E_{test}

$$\mathbb{E}[E_{valid}] = \mathbb{E}[E_{test}]$$

E_{valid} is an unbiased approximator of E_{test} …
… as long as it's evaluated only once.

$$E_{valid} = E_{test} + \epsilon$$

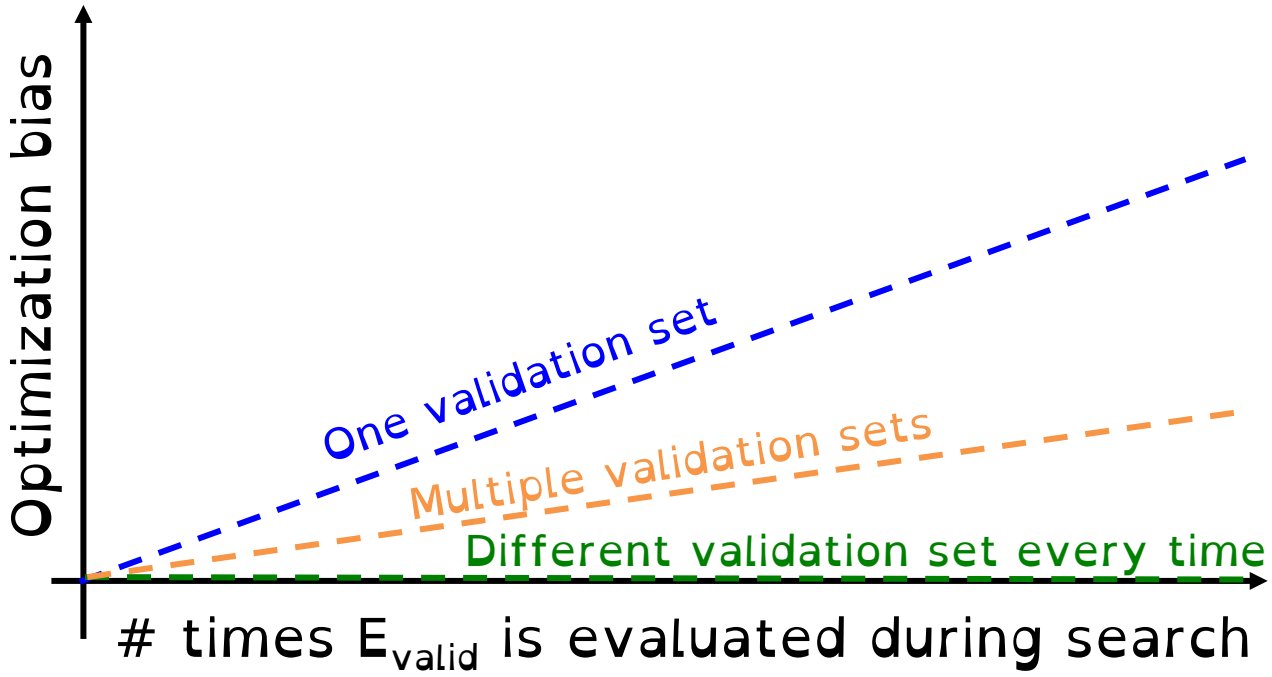
ϵ ← noise

$$\mathbb{E}[\epsilon] = 0$$

if E_{valid} is unbiased.

- The mean of error ϵ is a function of # of times you look at validation error

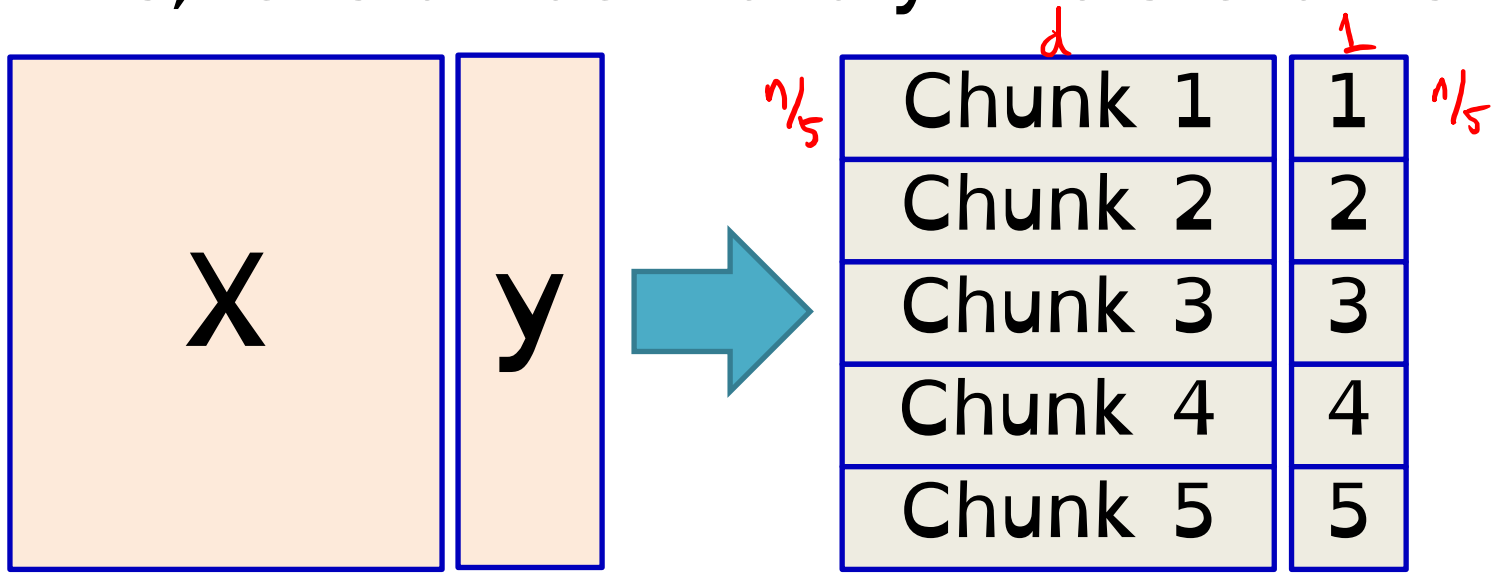
Recall: E_{valid} and E_{test}



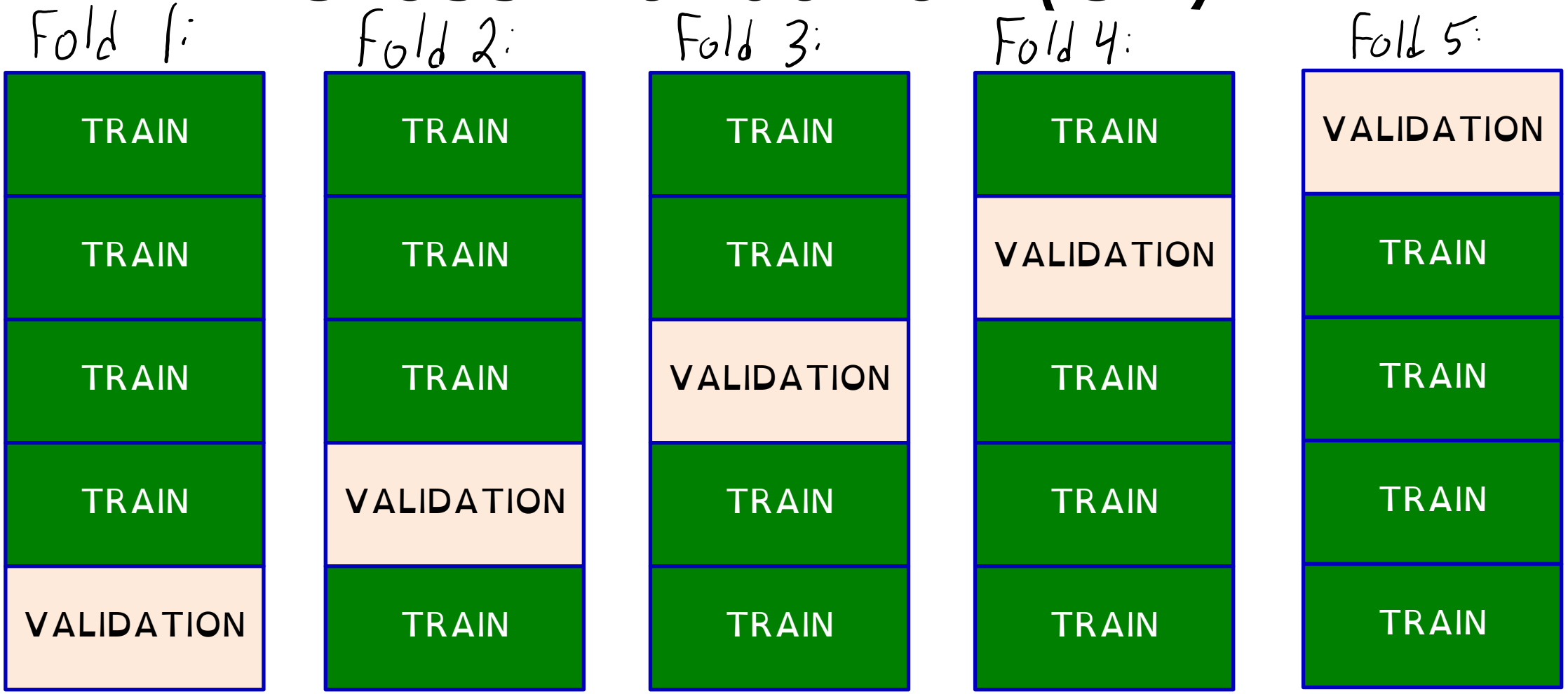
Cross-Validation (CV)

Q: How do we make multiple validation sets from the same training data?

- Idea: let's create multiple subsets of X and y.
  - 80% of data → training set X_{train} and y_{train}
  - 20% of data → validation set $X_{validate}$ and $y_{validate}$
  - We can do this split 5 times
- To do this, let's divide X and y into 5 chunks

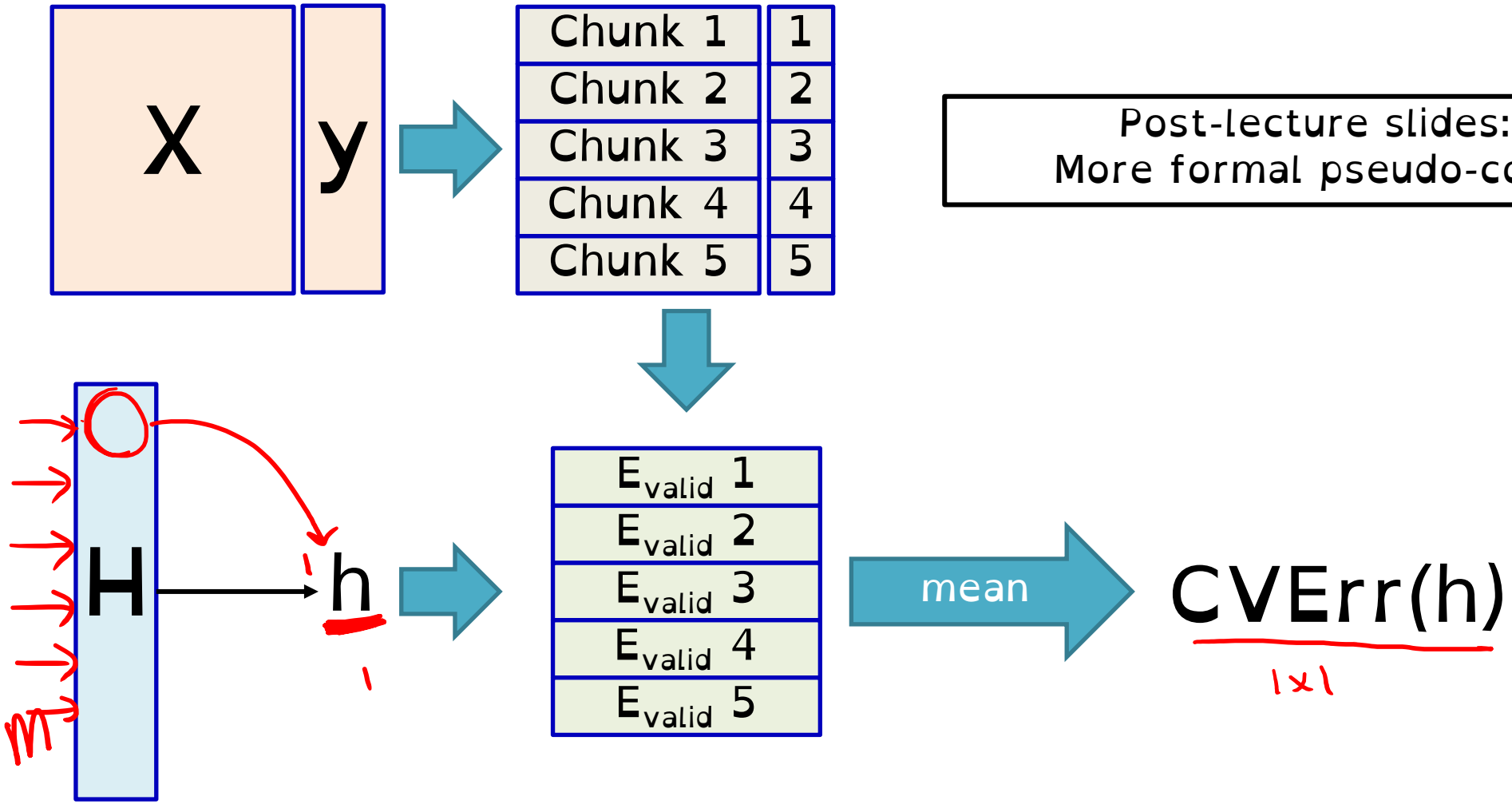


Cross-Validation (CV)



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

Hyper-Parameter Tuning with CV Pseudo-Code



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.
- Gets more accurate but more expensive with more folds.
  - To choose depth we compute the cross-validation score for each depth.

k=n

- As before, if data is ordered then folds should be random splits.
  - Randomize first, then split into fixed folds.

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.

Me waiting to hear about the best ML model so I can make lots of money

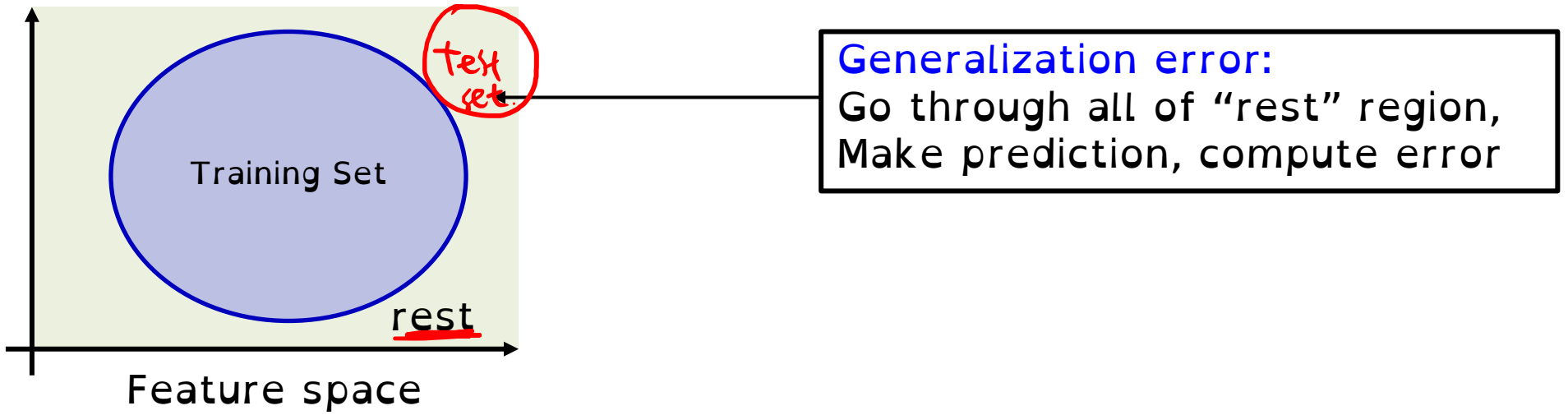
Coming Up Next

"BEST" MACHINE LEARNING MODEL

There is None

The "Best" Machine Learning Model

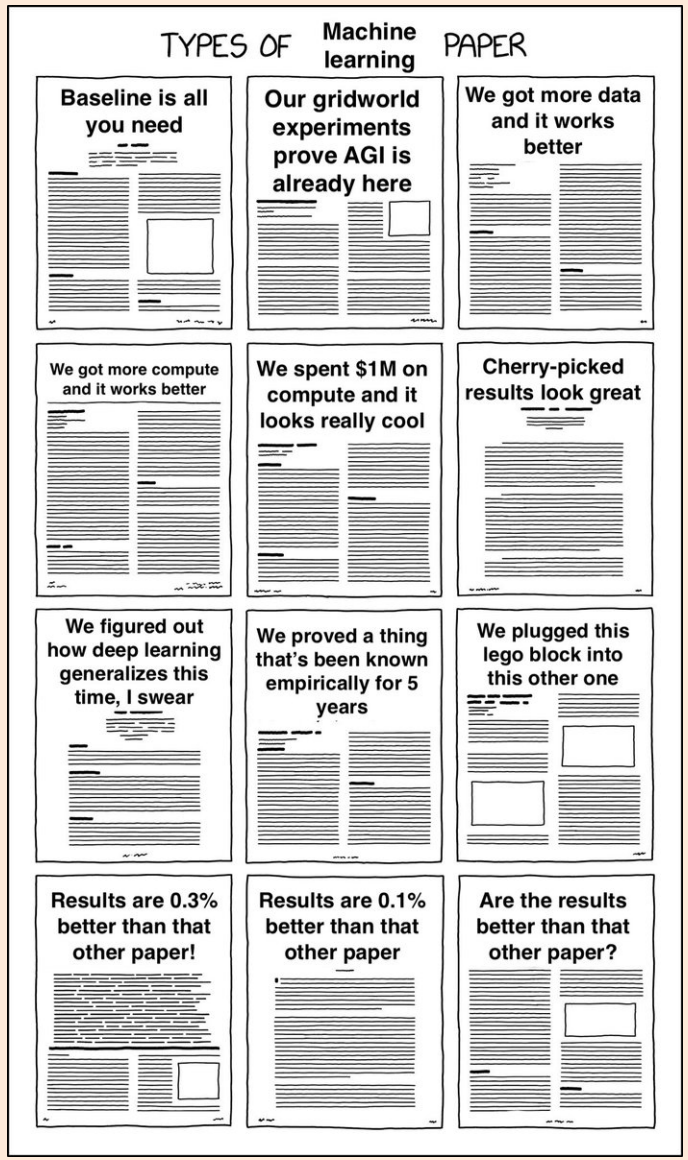
- Decision trees are not always most accurate on test error.
- What is the "best" machine learning model?
- An alternative measure of performance is the generalization error:
  - Average error over all x_i vectors that are not seen in the training set.
  - "How well we expect to do for a *completely unseen* feature vector".



The "Best" Machine Learning Model

- **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".
- Given a dataset, we need to 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.
- Machine learning research:
  - Large focus on models that are useful across many applications.

“State-Of-The-Art” Models



- A subset of ML research is OBSESSED with beating the state-of-the-art performance on benchmark tasks
  - State-of-the-art (SOTA)
    := test accuracy is best in the world
  - Benchmark tasks
    := well-known learning tasks
    (e.g. object recognition, machine translation, etc.)

- SOTA models for each task is very specialized.
  - Models that perform well on task A
    don’t necessarily perform well on task B

- Reviewers look carefully for whether your model works well across different datasets for the same task
  - Otherwise, you are not SOTA.
    You just overfitted to one dataset!

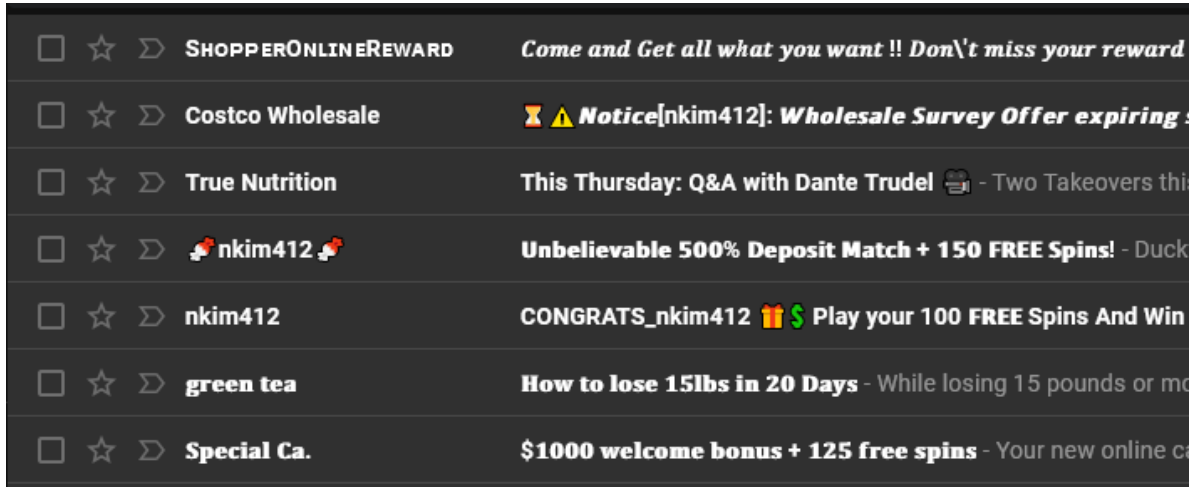
Coming Up Next

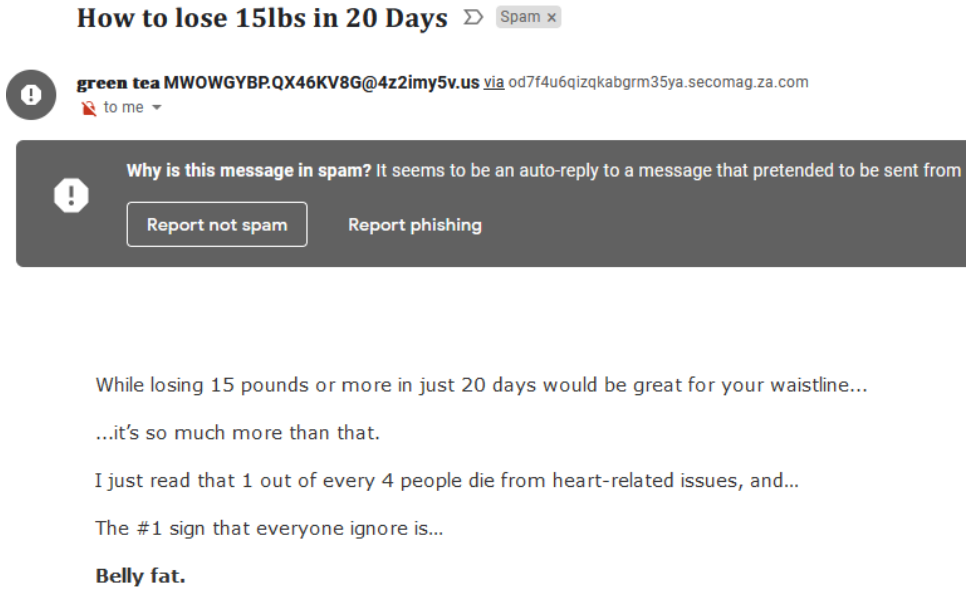
NAÏVE BAYES INTRO

Rev. Thomas Bayes

Application: Email Spam Filtering

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





Q: How do we formulate this as supervised learning?

Representing Emails

- Assumption: spam emails have a predictable pattern
  - Certain words occur more often in spams
    - E.g. “exclusive”, “offer”, “reward”, “Vicodin”, “keto”, etc.
  - Some words occur together more often in spams
    - E.g. “hi there”, “you have been selected”, “too late”, etc.
- We will represent emails with bag-of-words

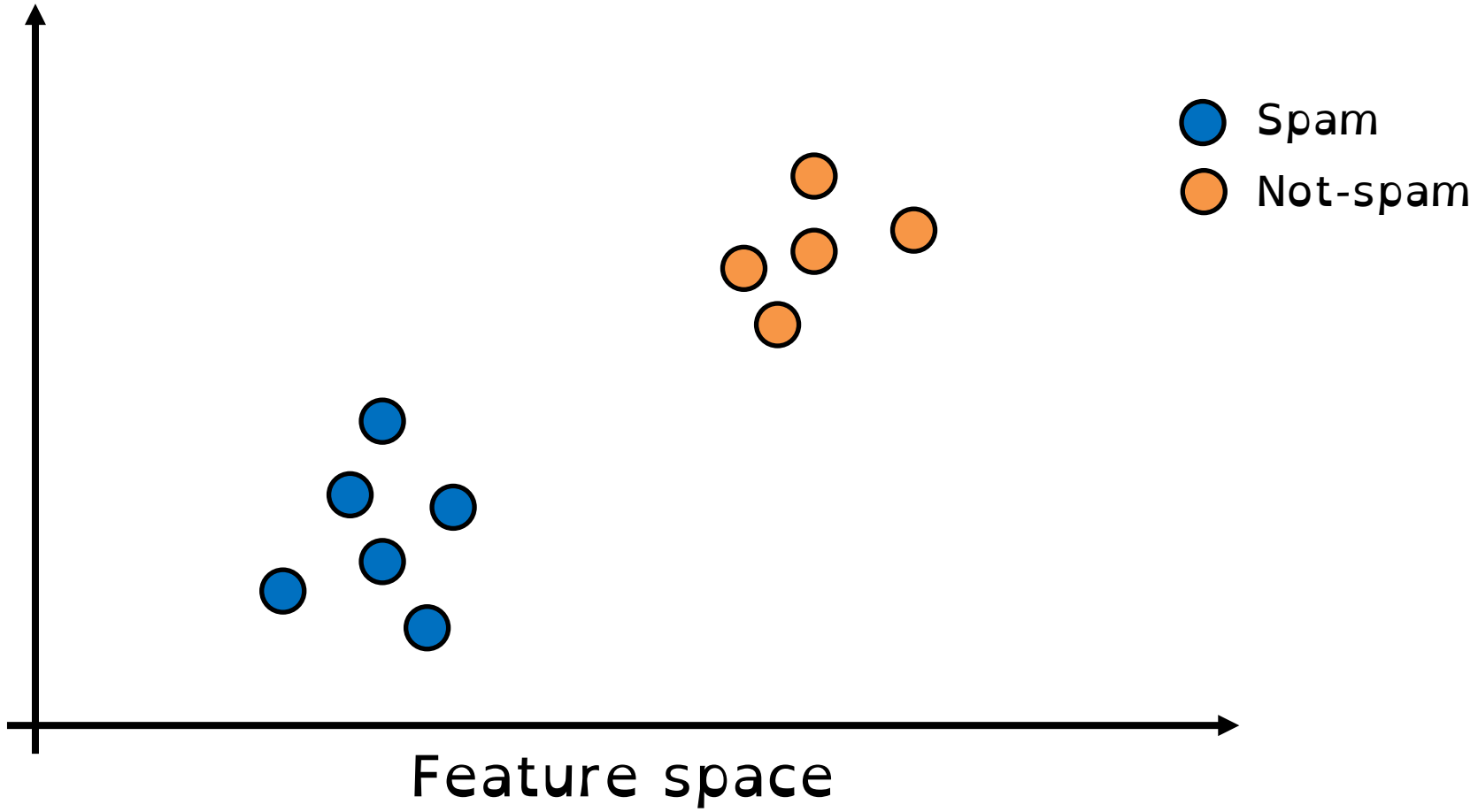
$	Hi	CPSC	340	Vicodin	Offer	…
1	1	0	0	1	0	…
0	0	0	0	1	1	…
0	1	1	1	0	0	…
…	…	…	…	…	…	…

d features: keywords for bag

- $x_{ij} = 1$ if word/phrase ‘j’ is in email ‘i’, $x_{ij} = 0$ if it is not.

Space of Emails

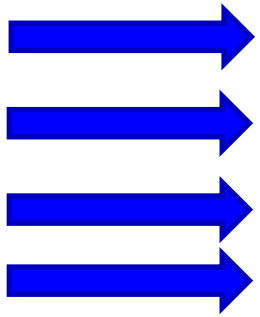
Spams have predictable patterns
=> spams and not-spams look different in space of emails



Spam Filtering as Supervised Learning

- Collect a large number of emails, gets user 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
…	…	…	…	…	…	…	…



- $y_i = 1$ if email ‘i’ is spam, $y_i = 0$ if email is not spam.

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: use probability for generating predictions
  - 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".

predict()

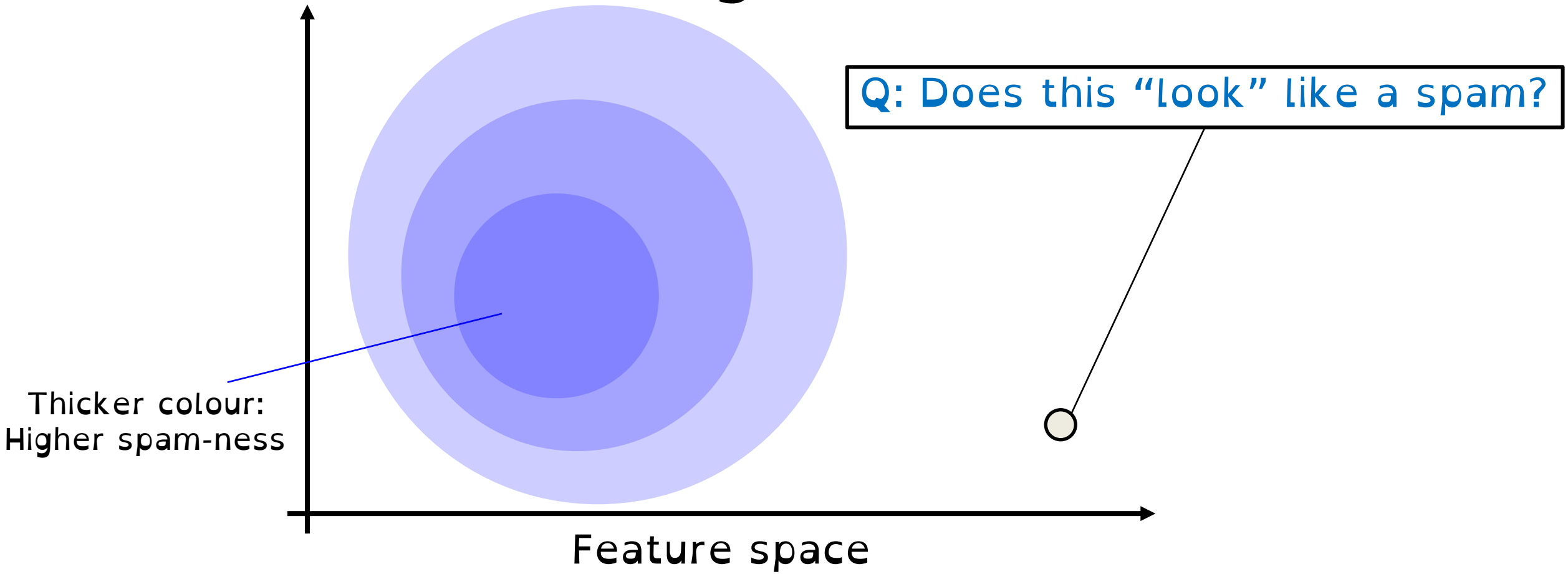
Note on Learned Probability

- $p(y_i = \text{“spam”} \mid x_i)$ reads:
  “probability that message is spam given these features”

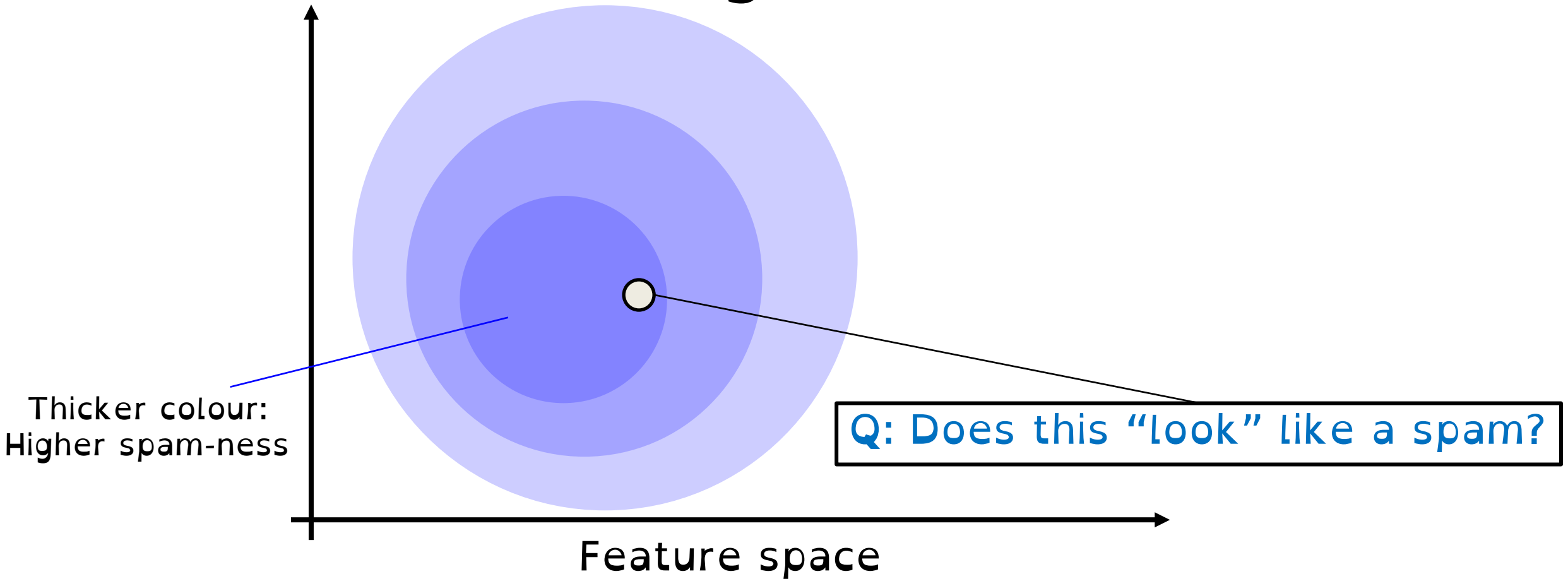
- In practice, we treat it more like a score:
  “the spam-ness of the input message”

- Our goal is to build a model that can compute the spam-ness, based on the examples of spam messages

Visualizing Spam-ness



Visualizing Spam-ness



Coming Up Next

NAÏVE BAYES DETAILS

Computing Spam-ness

$$p(y_i = \text{“spam”} \mid x_i)$$

- 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 email is spam.
  - Marginal probability $p(x_i)$ that an email 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.

Baseline:
- Performance
- I want to beat this performance.
- Super simple method.

What is $p(y_i)$?

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

- $p(y_i =$ "spam") is the "baseline spam-ness"
  - Probability that an email is a spam, without even looking at features.

Q: How do I learn this quantity?

Step 1: Look at all emails ~~in existence~~ in dataset (training)
Step 2: Count the number of spams

What is $p(x_i)$?

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

- $p(x_i)$ is the is probability that a random email looks like x_i

Q: How do I learn this quantity?

Step 1: Look at all emails ~~in existence~~ in dataset

Step 2: Count the number of times x_i occurs

What is $p(x_i \mid y_i)$?

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

- $p(x_i \mid y_i = \text{“spam”})$ is the is probability that a random spam looks like x_i

Q: How do I learn this quantity?

Step 1: Look at all **spams** ~~in existence~~ in dataset

Step 2: Count the number of times x_i occurs

IID Assumption

Too big to analyze

n is smaller but decently large

- IID assumption lets us treat the dataset as a snapshot of truth
  - i.e. emails in dataset (somewhat) accurately reflect the patterns in all emails in existence.
- Then probabilities can be estimated by frequencies in dataset

Counting for $p(x_i)$ and $p(x_i \mid y_i)$

- Seeing all possible examples at least once is extremely unlikely!

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

d features: keywords for bag

- I need to have $O(2^d)$ examples in order to see all possible examples.
- If I had fewer examples than that,
  I'll end up setting $p(x_i)$ and $p(x_i \mid y_i)$ to 0 all the time

Q: What should we do about that?

Getting Rid of $p(x_i)$

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

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 $p(x_i)$:

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

Naïve Bayes

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

$$p(x_i|y_i)$$

$$p(\text{hello}=1, \text{vicodin}=0, 340=1 \mid \text{spam}) \approx p(\text{hello}=1|\text{spam})\, p(\text{vicodin}=0|\text{spam})\, p(340=1|\text{spam})$$

HARD

easy easy 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").

What is p("Vicodin" = 0| y_i = "spam")?

$$p(hello=1, vicodin=0, 340=1 \mid spam) \approx p(hello=1 \mid spam)\, p(vicodin=0 \mid spam)\, p(340=1 \mid spam)$$

- p("vicodin" = 0| y_i = "spam") is the
  is probability that a spam does not contain the word "Vicodin"

Q: How do I learn this quantity?

Step 1: Look at all spams ~~in existence~~ in dataset

Step 2: Count the number of times "Vicodin" doesn't occur

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 ∞.

Review Questions

- Q1: Is having a super small search space always a good idea for hyper-parameter tuning?
- Q2: In practice, people rarely use cross-validation for very large datasets. Why?
- Q3: If we're using Naïve Bayes for spam filtering,
  why can a non-binary bag-of-words be problematic?
- Q4: What is so naïve about Naïve Bayes?

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

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>.

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.

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".

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.

Generalization Error

- An alternative measure of performance is the generalization error:
  - Average error over the set of x^i values that are not seen in the training set.
  - "How well we expect to do for a *completely unseen* feature vector".
- Test error vs. generalization error when labels are deterministic:

$$E_{test} = \mathbb{E}\left[|\hat{y}^i - \tilde{y}^i|\right]$$

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

$$E_{generalize} = \frac{1}{t}\sum_{x^i \notin \{train\ set\}} |\hat{y}_i - \tilde{y}_i|$$

number of x^i values not in training set.

average error over unseen x^i values.

“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.

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).

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.

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: $\{0,1\}^d$ -> $\{0,1\}$

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:
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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".