CSE 417T
Introduction to Machine Learning

Lecture 11

Instructor: Chien-Ju (CJ) Ho

Logistics

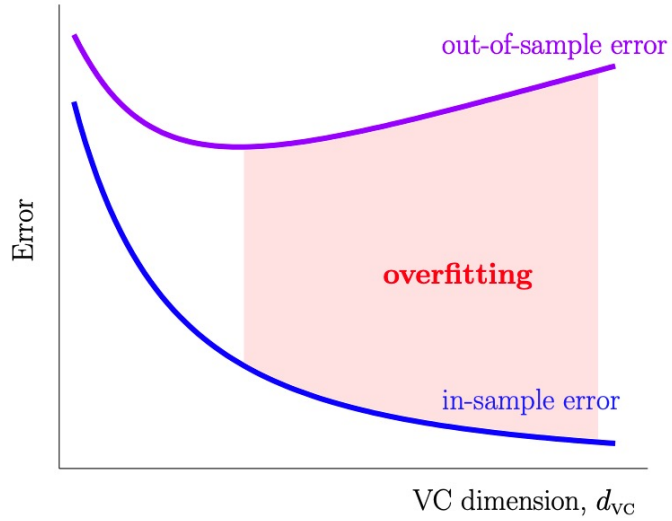
- Homework 2: Due **Feb 24** (Thu)
- Homework 3: Due **Mar 5** (Sat)
  - Keep track of your own late-day usages

- Exam 1: **Mar 10 (Thursday)**
  - Topics: LFD Chapters 1 to 5
  - Covid-permitting
    - Timed exam (75 min) during lecture time in the classroom
    - Closed-book exam with 2 letter-size cheat sheets allowed (4 pages in total)
      - No format limitations (it can be typed, written, or a combination)
  - Mar 8 (Tuesday) will be a review lecture

Recap

Overfitting and Its Cures

- Overfitting
  - Fitting the data more than is warranted
  - Fitting the noise instead of the pattern of the data
  - Decreasing E_{in} but getting larger E_{out}
  - When H is too strong, but N is not large enough



- Regularization
  - Intuition: Constrain H to make overfitting less likely to happen

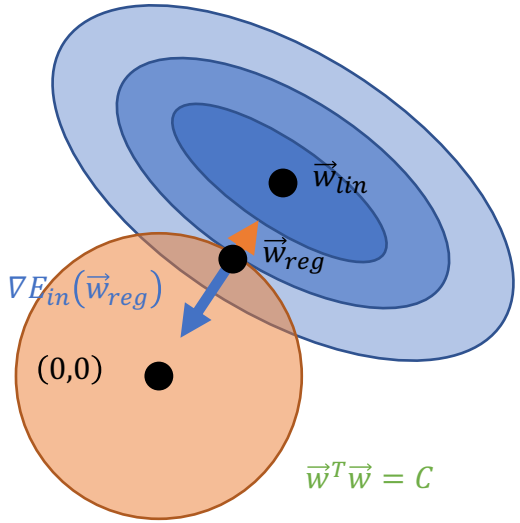
- Validation
  - Intuition: Reserve data to estimate E_{out}

Regularization (Constrain H)

- Weight decay

$$H(C) = \{h \in H_Q \text{ and } \vec{w}^T\vec{w} \leq C\}$$

- Algorithm: Find $g \in H(C)$ such that $g \approx f$



Constrained optimization

minimize $E_{in}(\vec{w})$

subject to $\vec{w}^T\vec{w} \leq C$

equivalent

Unconstrained optimization

minimize $E_{in}(\vec{w}) + \frac{\lambda_C}{N}\vec{w}^T\vec{w}$

Augmented error

Augmented Error

$$E_{aug}(h, \lambda, \Omega) = E_{in}(\vec{w}) + \frac{\lambda}{N}\Omega(h)$$

- Key components
  - Ω: Regularizer
  - λ: Amount of regularization

- Does the form look familiar? Recall in the VC Theory (treating δ as a constant)
  - $E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{vc}\frac{\ln N}{N}}\right)$

- What the impacts of picking Ω and λ?

Summary of Regularization

- Regularization is everywhere in machine learning

- Two main ways of thinking about regularization
  - Constrain H to make overfitting less likely to happen
    - Will discuss more regularization methods in the 2nd half of the semester
    - Pruning for decision trees, early stopping / dropout for neural networks, etc
  - Define augmented error E_{aug} to better approximate E_{out}
    - $E_{aug}(h, \lambda, \Omega) = E_{in}(\vec{w}) + \frac{\lambda}{N}\Omega(h)$

- We show the equivalence of the two for weight decay
  - The conceptual equivalence is general with Lagrangian relaxation (will cover later in the semester)

Today’s Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

Let me know if you spot errors.

Prevent Overfitting

$$E_{out}(g) = E_{in}(g) + \text{overfit penalty}$$

- Regularization
  - Choose a regularizer Ω to approximate the penalty
- Validation
  - Directly estimate E_{out} (The goal of learning is to minimize E_{out})

Review of Test Set (Estimate E_{out})

- Out-of-sample error $E_{out}(g) = \mathbb{E}_{\vec{x}}[e(g(\vec{x}), y)]$
  - Key: $\vec{x}$ need to be out of sample (i.e., not in training)

- Test set $D_{test} = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_K, y_K)\}$
  - Reserve K data points
  - None of the data points in test set can be involved in training

- Using the data in test set to estimate E_{out}
  - Since all data points in D_{test} are out of sample

Short Discussion on HW2

- In HW2, you are asked to perform “normalization” on the training/test datasets. How should you do it?

    1. Calculate the mean/variance of the combined data.
       Normalize them using the overall mean/variance.
    2. Calculate the means/variances of training and test datasets separately.
       Normalize them using their respective mean/variance.
    3. Calculate the mean/variance of training dataset.
       Normalize both datasets using the training mean/variance.

Short Discussion on HW2

- In HW2, you are asked to perform “normalization” on the training/test datasets. How should you do it?

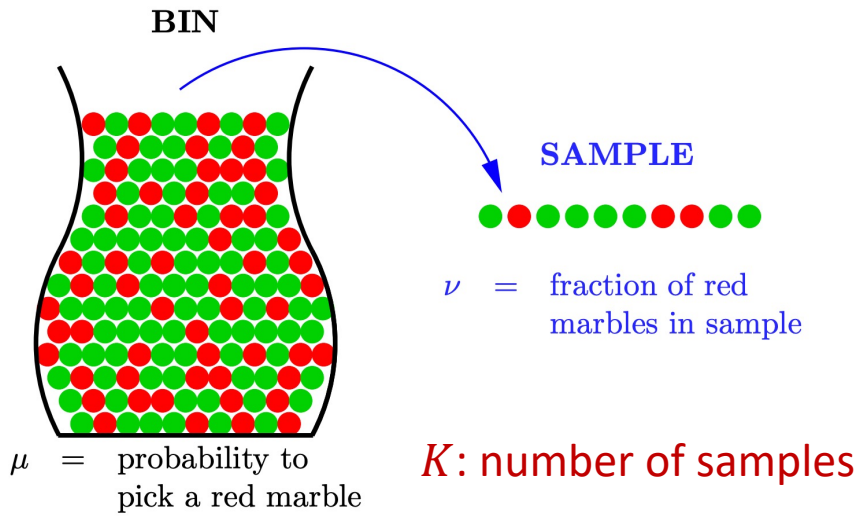
1. Calculate the mean/variance of the combined data.
   Normalize them using the overall mean/variance.
2. Calculate the means/variances of training and test datasets separately.
   Normalize them using their respective mean/variance.
3. Calculate the mean/variance of training dataset.
   Normalize both datasets using the training mean/variance.

Two important properties we want to preserve
1. Training and test data are drawn from the same distribution.
2. Test data is never used in training.

Test Set

- Test set $D_{test} = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_K, y_K)\}$
- For a g learned using only training set
  - g is a "fixed" hypothesis for D_{test}

- Let $E_{test}(g) = \frac{1}{K}\sum_{k=1}^{K} e(g(\vec{x}_k), y_k)$
  - $E_{test}(g)$ is an unbiased estimate of $E_{out}(g)$
    - $\mathbb{E}[E_{test}(g)] = \frac{1}{K}\sum_{k=1}^{K} \mathbb{E}[e(g(\vec{x}_k), y_k)] = E_{out}(g)$
  - Single-hypothesis Hoeffding bound applies
    - $E_{out}(g) \leq E_{test}(g) + O\left(\sqrt{\frac{1}{K}}\right)$

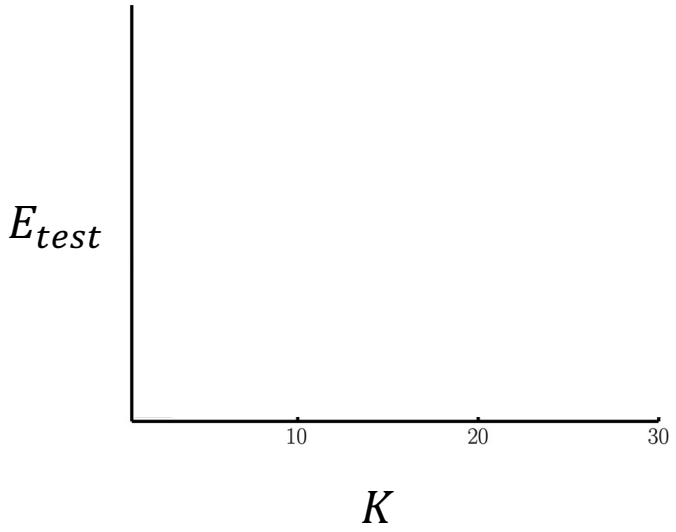


K: number of samples

Where are Test Set From?

- Given a data set D of N points
  - $D = D_{train} \cup D_{test}$
  - Reserving K points for test set means we only have $N - K$ points for training

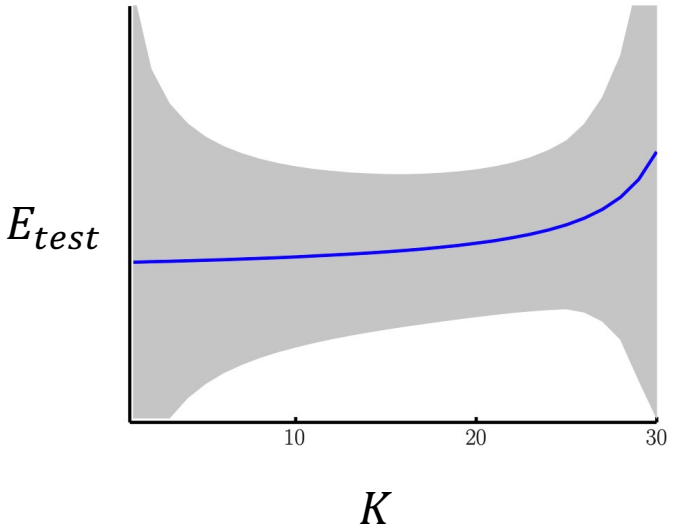
- Effect of the choice of K



Where are Test Set From?

- Given a data set D of N points
  - $D = D_{train} \cup D_{test}$
  - Reserving K points for test set means we only have $N - K$ points for training

- Effect of the choice of K



Rule of Thumb: $K^* = \frac{N}{5}$

Utilizing the Whole D

- Process:
  - $D = D_{train} \cup D_{test}$ where $|D_{test}| = K, |D_{train}| = N - K$
  - Learn some hypothesis g^- using only D_{train}
  - Estimate $E_{out}(g^-)$ using D_{test}
- Can we do better than g^- ?
  - Yes! Learn g using the entire D; return g and $E_{test}(g^-)$
- Generally (Informal, not theoretically proven)
  - Training on more data leads to better learned hypothesis
  - $E_{out}(g) \leq E_{out}(g^-)$

Validation: Beyond Test Set

What if we want to estimate E_{out} multiple times?

Validation: Beyond Test Set

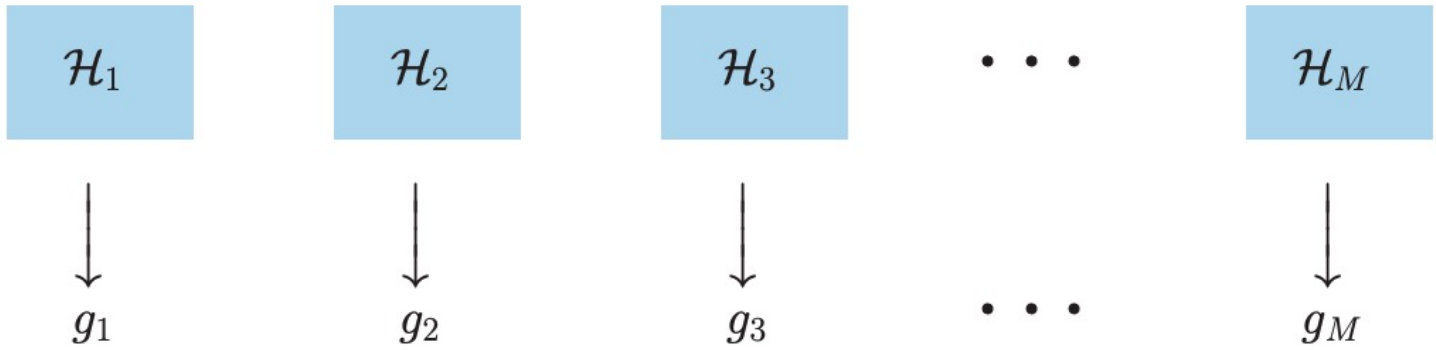
- Model selection:
  - Should I use linear models or decision trees?
  - Should I set the regularization parameter λ to 0.1, 0.01, or 0.001?
    - A model with different λ can be considered as different model

- Validation set
  - $D = D_{train} \cup D_{val}$

  - Key difference to the test set
    - D_{val} could be used multiple times for model selection
    - We need to account for the multiple usages of D_{val}

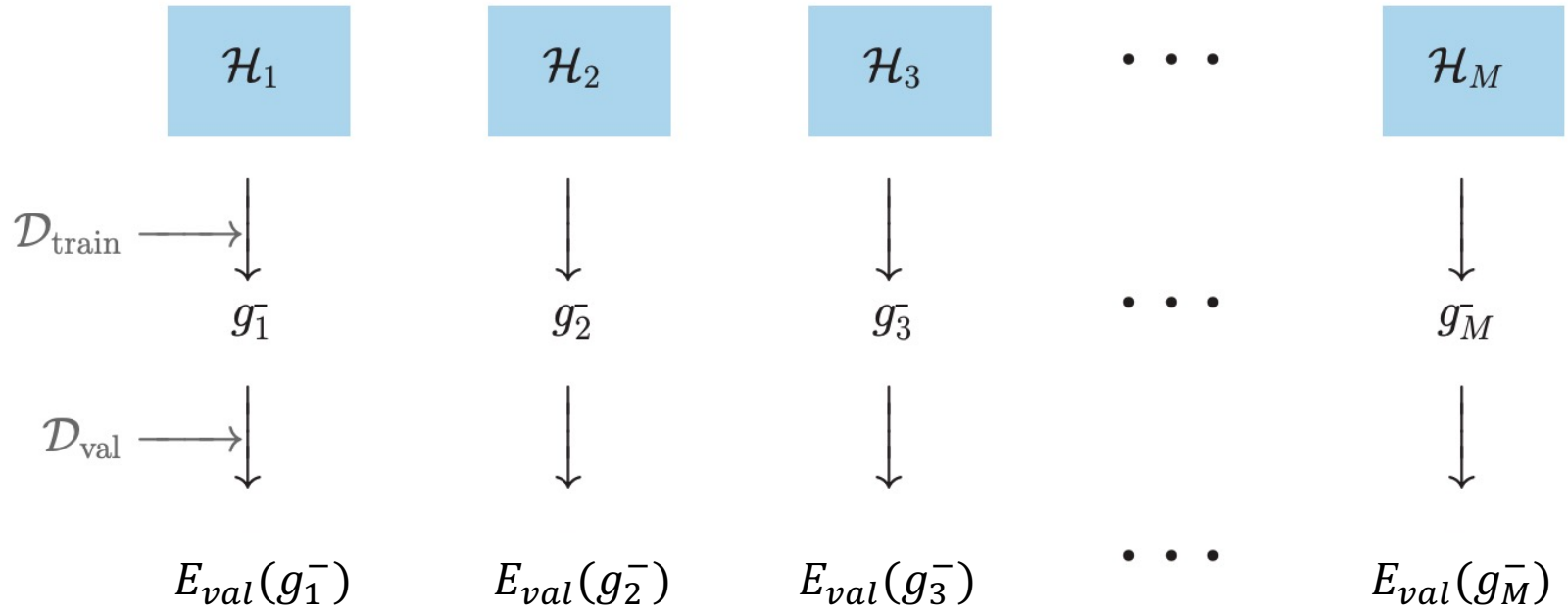
Model Selection

- Which model should we choose?



Model Selection using Validation

- Which model should we choose?



Key: D_{val} is used to choose from M hypothesis

Choose H_{m^*} such that $E_{val}(g_{m^*}^-) \leq E_{val}(g_m^-)$ for all m

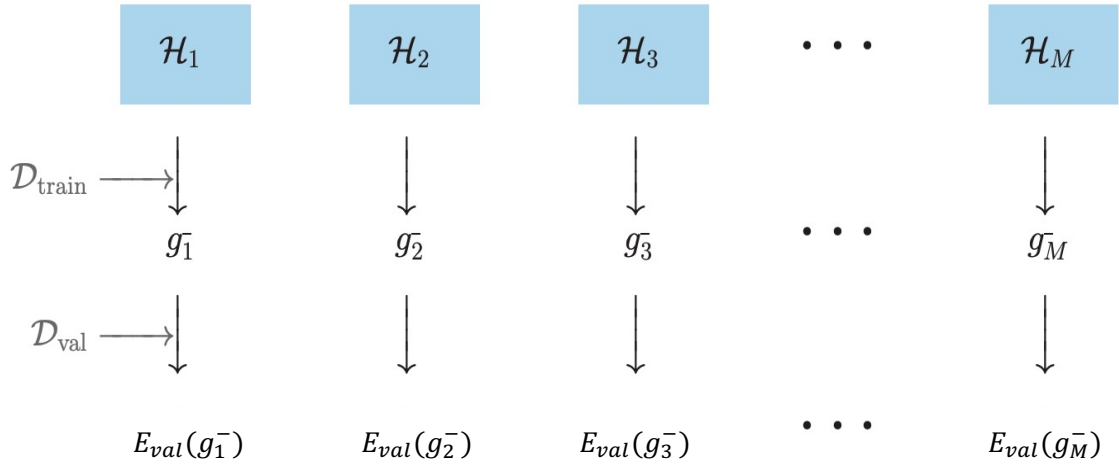
Question…

- Which of the following is true?

(a) $\mathbb{E}[E_{val}(g_{m^*}^-)] = E_{out}(g_{m^*}^-)$

(b) $\mathbb{E}[E_{val}(g_{m^*}^-)] \leq E_{out}(g_{m^*}^-)$

(c) $\mathbb{E}[E_{val}(g_{m^*}^-)] \geq E_{out}(g_{m^*}^-)$



Choose H_{m^*} such that $E_{val}(g_{m^*}^-) \leq E_{val}(g_m^-)$ for all m

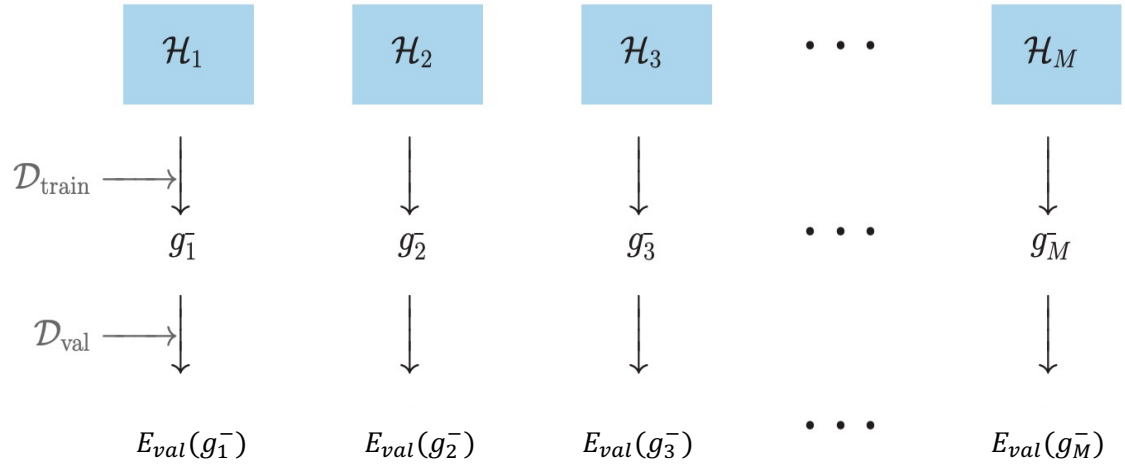
Question…

- Which of the following is true?

(a) $\mathbb{E}[E_{val}(g_{m^*}^-)] = E_{out}(g_{m^*}^-)$

(b) $\mathbb{E}[E_{val}(g_{m^*}^-)] \leq E_{out}(g_{m^*}^-)$

(c) $\mathbb{E}[E_{val}(g_{m^*}^-)] \geq E_{out}(g_{m^*}^-)$



Choose H_{m^*} such that $E_{val}(g_{m^*}^-) \leq E_{val}(g_m^-)$for all m

Equivalent to use D_{val} to choose from $H = \{g_1^-, \ldots, g_M^-\}$

$$E_{out}(g_{m^*}^-) \leq E_{val}(g_{m^*}^-) + O\left(\sqrt{\frac{\ln M}{K}}\right)$$ => Hoeffding Bound for Multiple Hypothesis

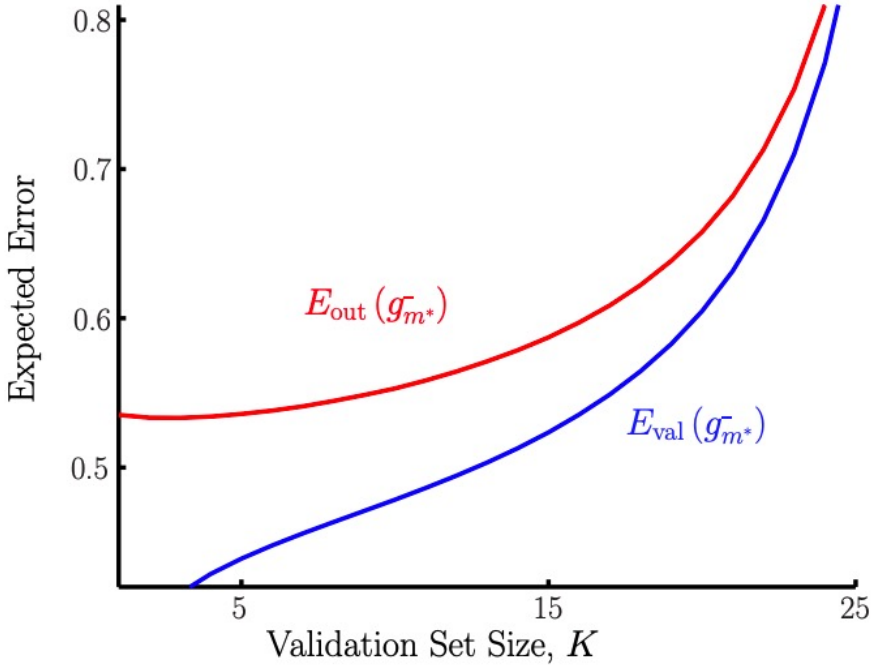
Question…

- Which of the following is true?

(a) $\mathbb{E}[E_{val}(g_{m^*}^-)] = E_{out}(g_{m^*}^-)$

(b) $\mathbb{E}[E_{val}(g_{m^*}^-)] \leq E_{out}(g_{m^*}^-)$

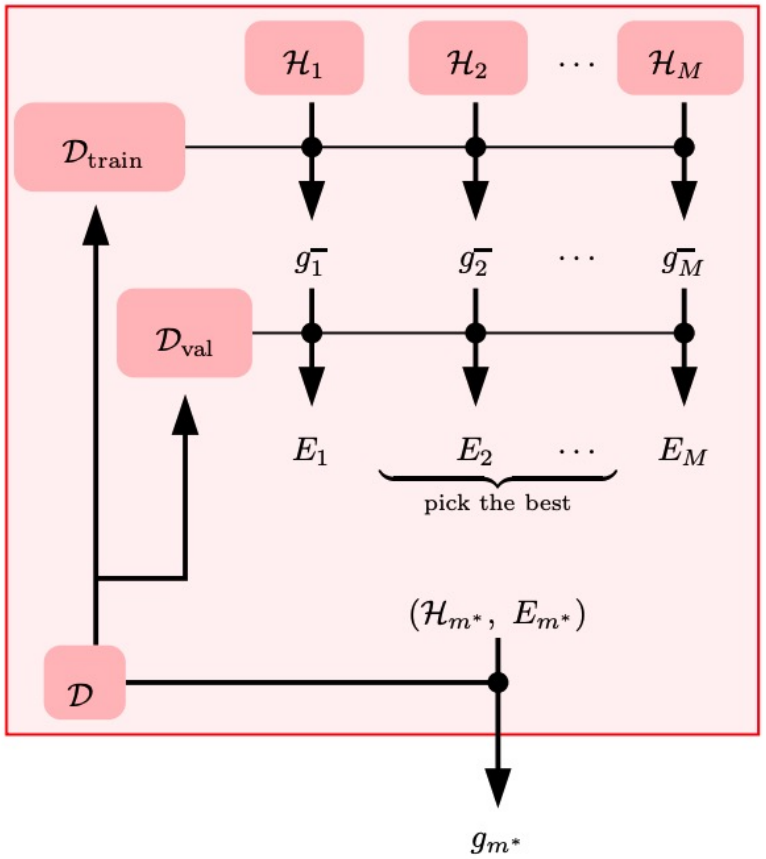
(c) $\mathbb{E}[E_{val}(g_{m^*}^-)] \geq E_{out}(g_{m^*}^-)$

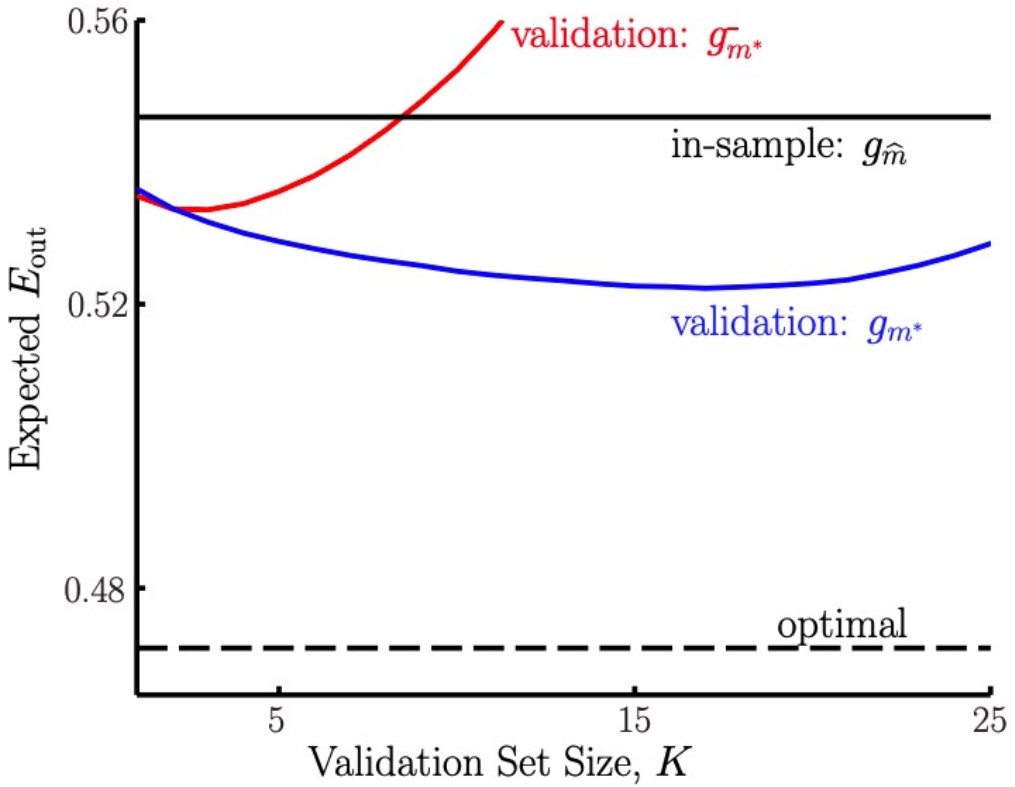


Equivalent to use D_{val} to choose from $H = \{g_1^-, \ldots, g_M^-\}$

$$E_{out}(g_{m^*}^-) \leq E_{val}(g_{m^*}^-) + O\left(\sqrt{\frac{\ln M}{K}}\right)$$ => Hoeffding Bound for Multiple Hypothesis

Utilizing the Whole D





$g_{\widehat{m}}$: the hypothesis minimizes in-sample error over $\{H_1, \ldots, H_M\}$

	Outlook	Relationship to E_{out}
E_{in}		
E_{val} (when used for model selection)		
E_{test}		

When a validation set is not used for model selection (i.e., used only once), it is essentially a test set

	Outlook	Relationship to E_{out}
E_{in}	Incredibly optimistic	
E_{val} (when used for model selection)	Slightly optimistic	
E_{test}	Unbiased	

	Outlook	Relationship to E_{out}
E_{in}	Incredibly optimistic	VC-bound
E_{val} (when used for model selection)	Slightly optimistic	Hoeffding's bound (multiple hypotheses)
E_{test}	Unbiased	Hoeffding's bound (single hypothesis)

Note that the outlook comparisons are "in expectation"
If you only get one "draw" of $D_{train}, D_{val}, D_{test}$, you cannot say anything "for certain"

Remember that ML results are under the condition "with high probability"

The Dilemma When Choosing K

- The main ideas behind validation

Want large K
(E_{val} estimates E_{out} well)

$$E_{out}(g) \approx E_{out}(g^-) \approx E_{val}(g^-)$$

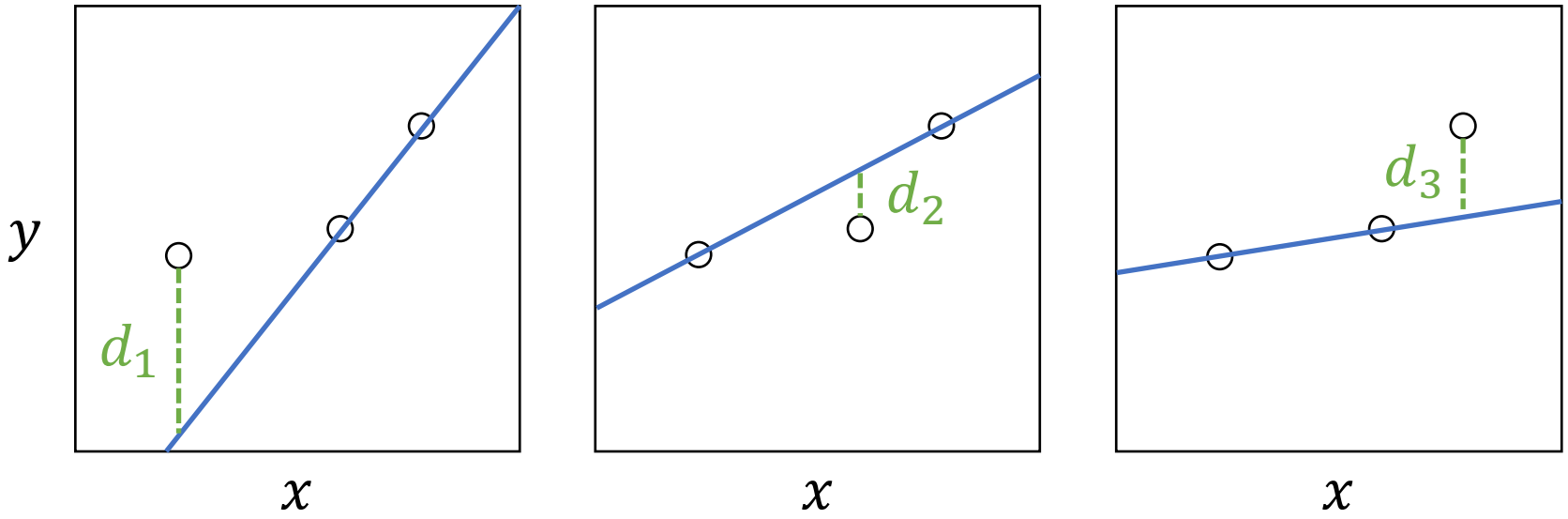
Want small K
(didn't sacrifice too much training data)

Leave-One-Out Cross Validation (LOOCV)

Getting the best of both worlds

Intuition: Setting $K = 1$ but do it many times…

Illustrative Example



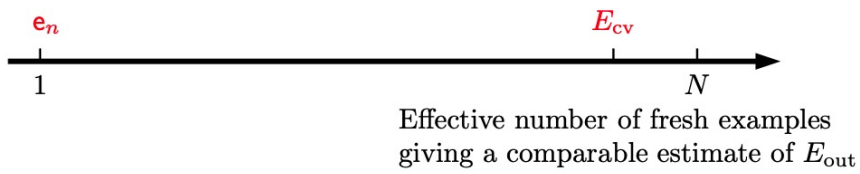
$$E_{cv} = \frac{1}{3}(d_1^2 + d_2^2 + d_3^2)$$

Properties of LOOCV

- LOOCV is unbiased (If *not* used for model selection)
  - E_{CV} is an unbiased estimator of $\bar{E}_{out}(N-1)$

(expected E_{out} when learning on $N-1$ points)

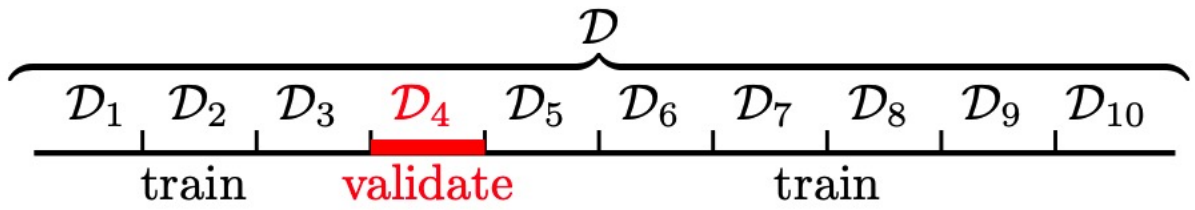
- The "effective number" of examples in E_{CV} estimation is high for LOOCV



- However, LOOCV is computationally expensive
  - Need to train N models, each on $N-1$ points

V-Fold Cross Validation

- Split D into V equally sized data sets: $D_1, D_2, \ldots, D_V$
  - Let g_i^- be the hypothesis learned using all data sets except D_i
  - Let $e_i = E_{val}(g_i^-)$ where the validation uses data set D_i
- The V-fold cross validation error is $\frac{1}{V}\sum_{i=1}^{V} e_i$



- Practical rule of thumb: $V = 10$

Three Learning Principles

Occam’s Razor

Sampling Bias

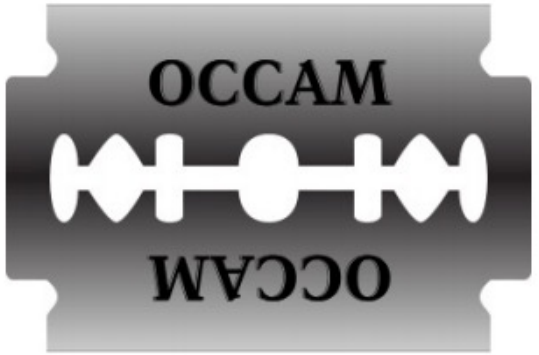
Data Snooping

Occam's Razor

"An explanation of the data should be made as simple as possible, but no simpler."
-- Einstein?

"entia non sunt multiplicanda praeter necessitatem"
(entities must not be multiplied beyond necessity)
-- William of Occam

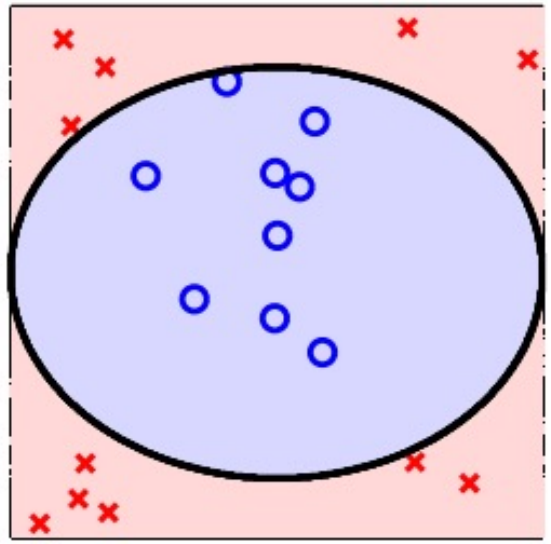
"trimming down"
unnecessary explanation

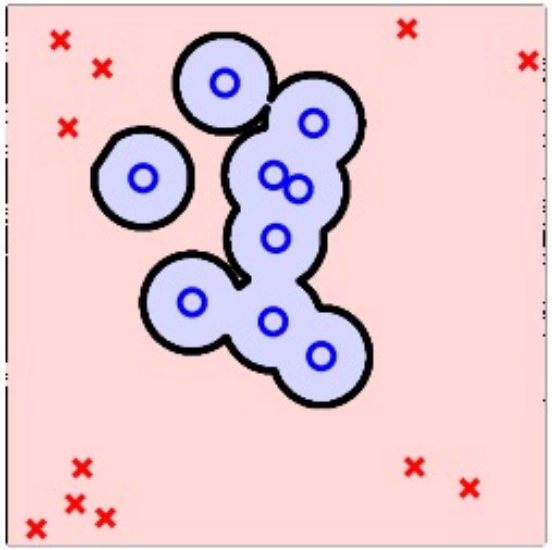


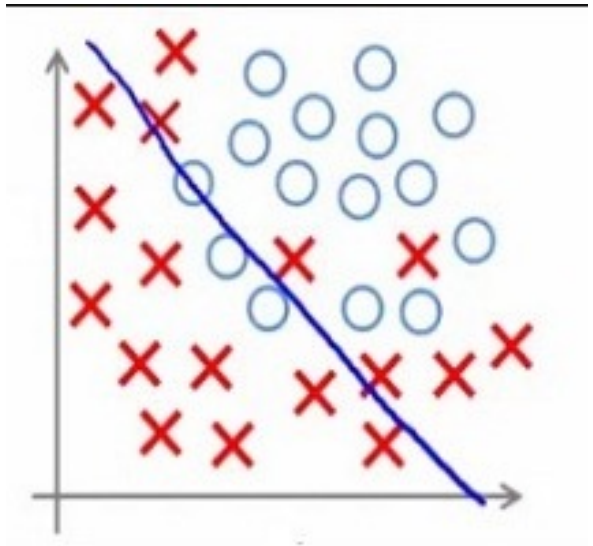
The simplest model that fits the data is also the most plausible

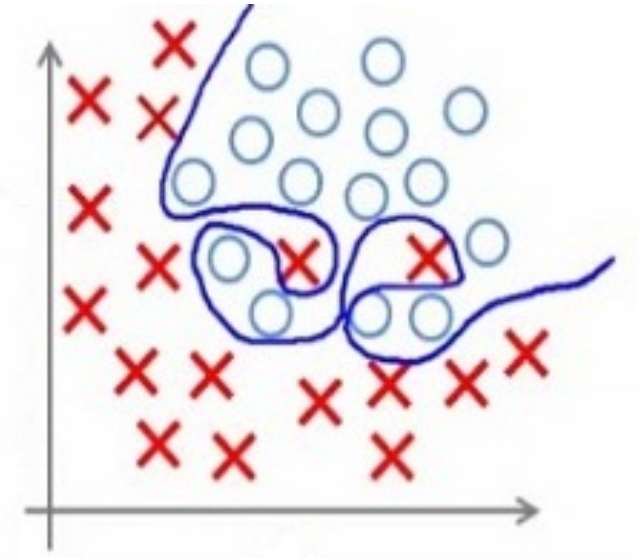
What does it mean to be simple?

Why is simple better?









Simple Model?

- For a hypothesis set H to be simple
  - # dichotomies it can generate is small
  - VC Dimension is small

- For a hypothesis h to be simple
  - lower order polynomial
  - smaller weights (think about the regularization)
  - easy to describe?
  - fewer number of parameters (fewer bits to describe)

Simple Model?

Connection:

A hypothesis set with *simple* hypotheses should be *simple*

Consider a hypothesis h can be specified by ℓ bits

$\Rightarrow H$ contains all such h

$\Rightarrow$ The size of H is 2^{ℓ}

Simple: small model complexity / VC dimension / size of hypothesis set

Why is Simple Better?

simple -> small VC dimension -> good generalization, less overfitting, …

Simple $\mathcal{H}$

$\Rightarrow$ small growth function $m_{\mathcal{H}}(N)$

$\Rightarrow$ if data labels are generated randomly, the probability of fitting perfectly is?

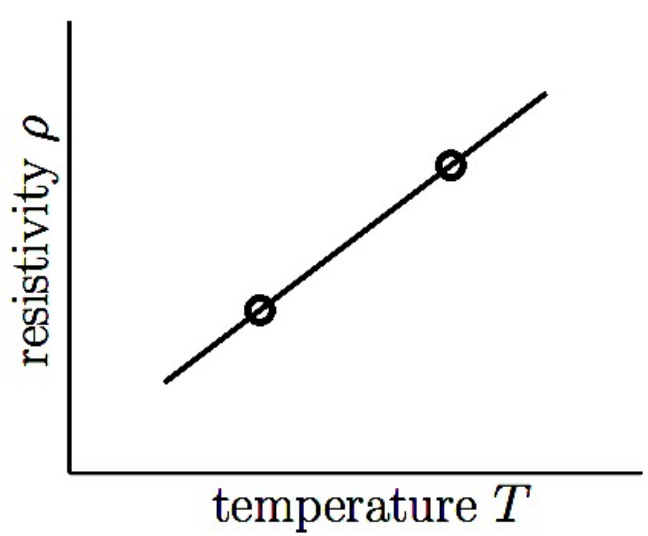
$$\frac{m_{\mathcal{H}}(N)}{2^N}$$

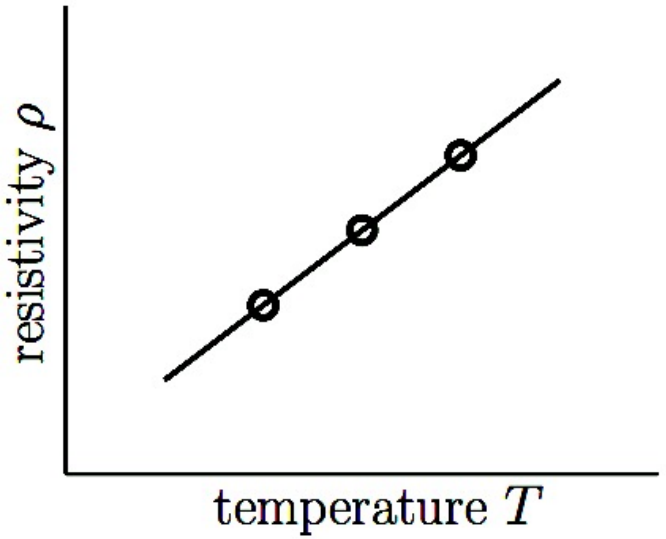
$\Rightarrow$ more significant when fit really happens

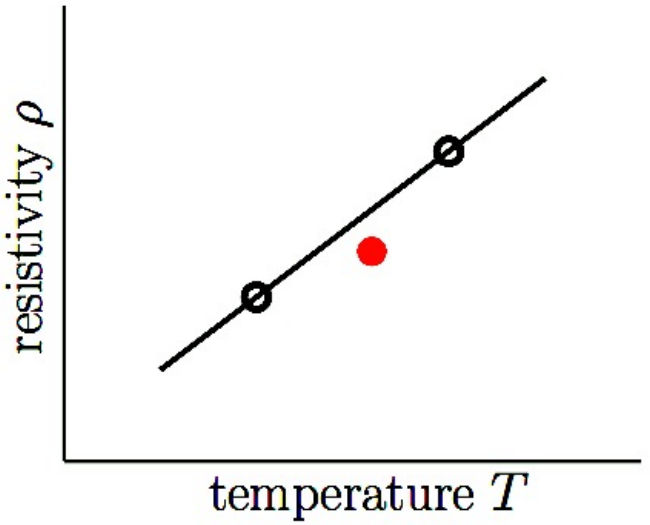
Falsifiability is important!

Falsifiability

Say you want to examine whether resistivity is linear in temperature (assume no measure error)







A Classical Puzzle

Imagine you got an email before each Cardinals game for the first 5 games.

Before Game 1: “Cardinals will win” -> Cardinals wins Game 1
Before Game 2: ”Cardinals will lose” -> Cardinals loses Game 2
….

Before Game 6:
If you pay me $50 dollars, I’ll tell you whether Cardinals will win or not

It’s not falsifiable:
Imagine if this person contacts 2^{10} persons, split them into two groups each game
2^5 persons will receive perfect prediction for the first 5 games

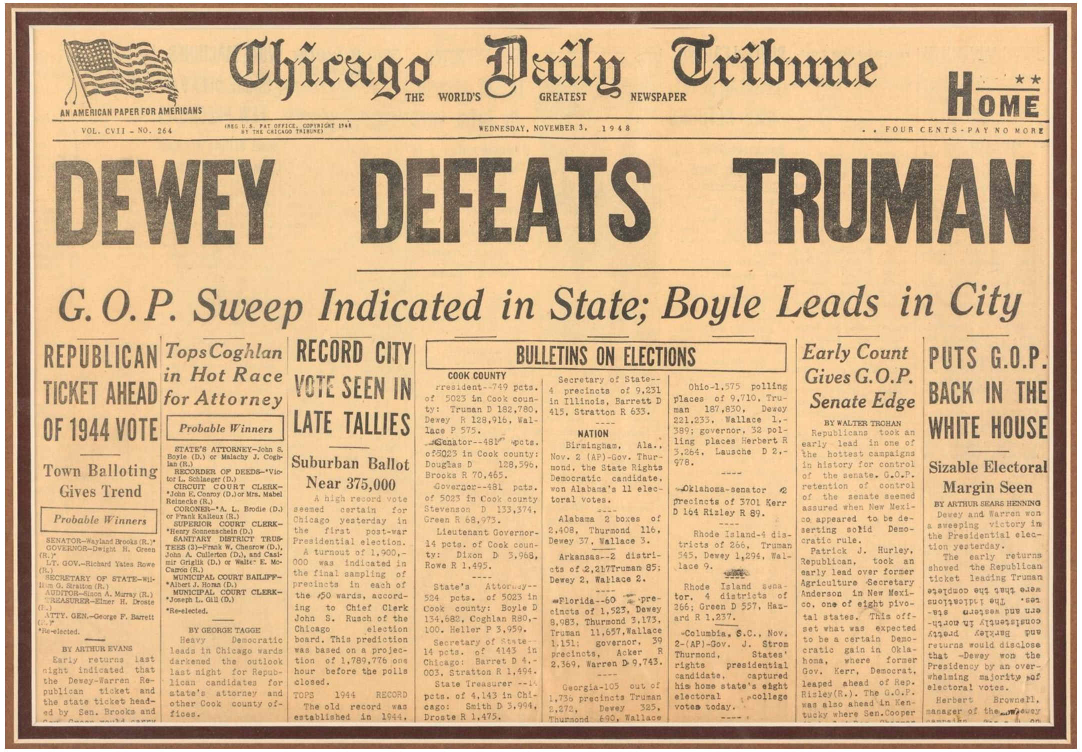
Occam’s Razor

Sampling Bias

Data Snooping

1948 US Presidential Election

- Truman vs. Dewey
- Chicago Daily Tribune decided to run a phone poll of how people <u>voted</u>



Chicago Daily Tribune
THE WORLD'S GREATEST NEWSPAPER
AN AMERICAN PAPER FOR AMERICANS
HOME
VOL. CVII - NO. 264
WEDNESDAY, NOVEMBER 3, 1948
FOUR CENTS-PAY NO MORE

DEWEY DEFEATS TRUMAN

G. O. P. Sweep Indicated in State; Boyle Leads in City

REPUBLICAN TICKET AHEAD OF 1944 VOTE
Town Balloting Gives Trend
Probable Winners

Tops Coghlan in Hot Race for Attorney
Probable Winners

RECORD CITY VOTE SEEN IN LATE TALLIES
Suburban Ballot Near 375,000

BULLETINS ON ELECTIONS

Early Count Gives G.O.P. Senate Edge
BY WALTER TROHAN

PUTS G.O.P. BACK IN THE WHITE HOUSE
Sizable Electoral Margin Seen
BY ARTHUR SEARS HENNING

Truman


Chicago Daily Tribune
DEWEY DEFEATS TRUMAN
G.O.P. Sweep Indicated in State; Boyle Leads in

What happened?

One explanation: we cannot claim anything for certain.

However, there are bigger issues here…

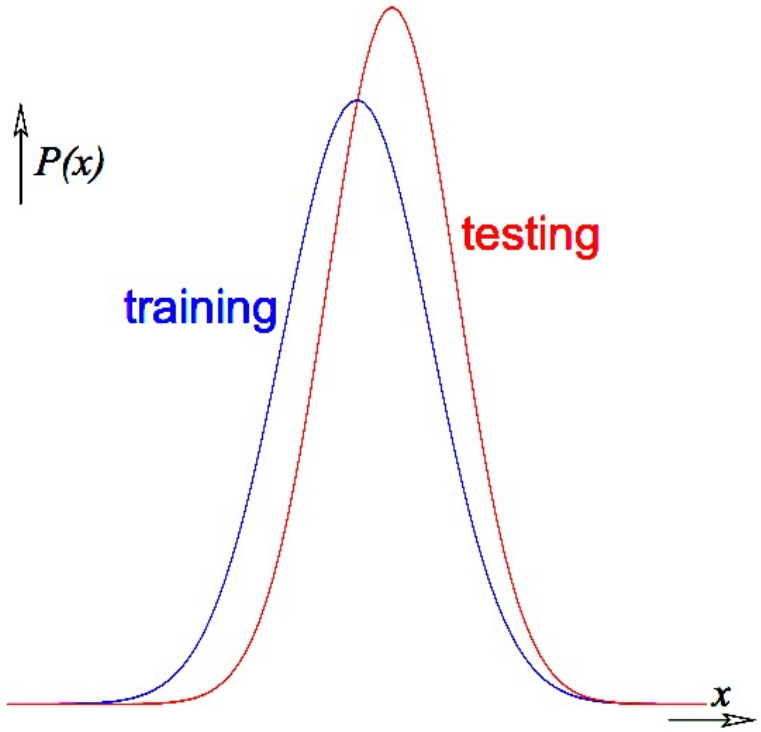
- Phones are expensive in 1948…
- Dewey was more favored in rich populations

- Imagine you are polling from people in DC/Texas/NY to predict who will win the presidential election…

Sampling Bias

If the data is sampled in a biased way, learning will produce a similarly biased outcome.

What can we do….

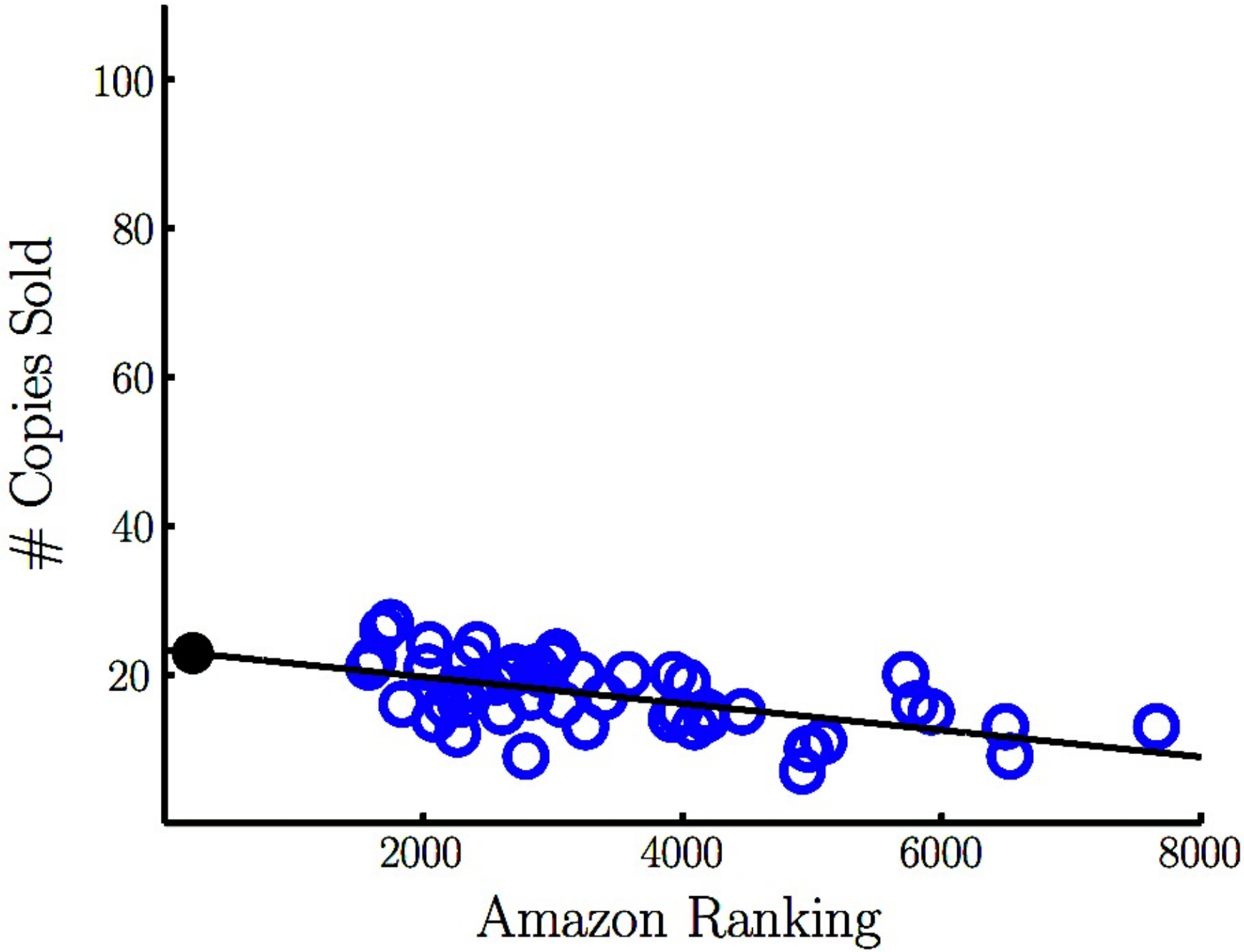


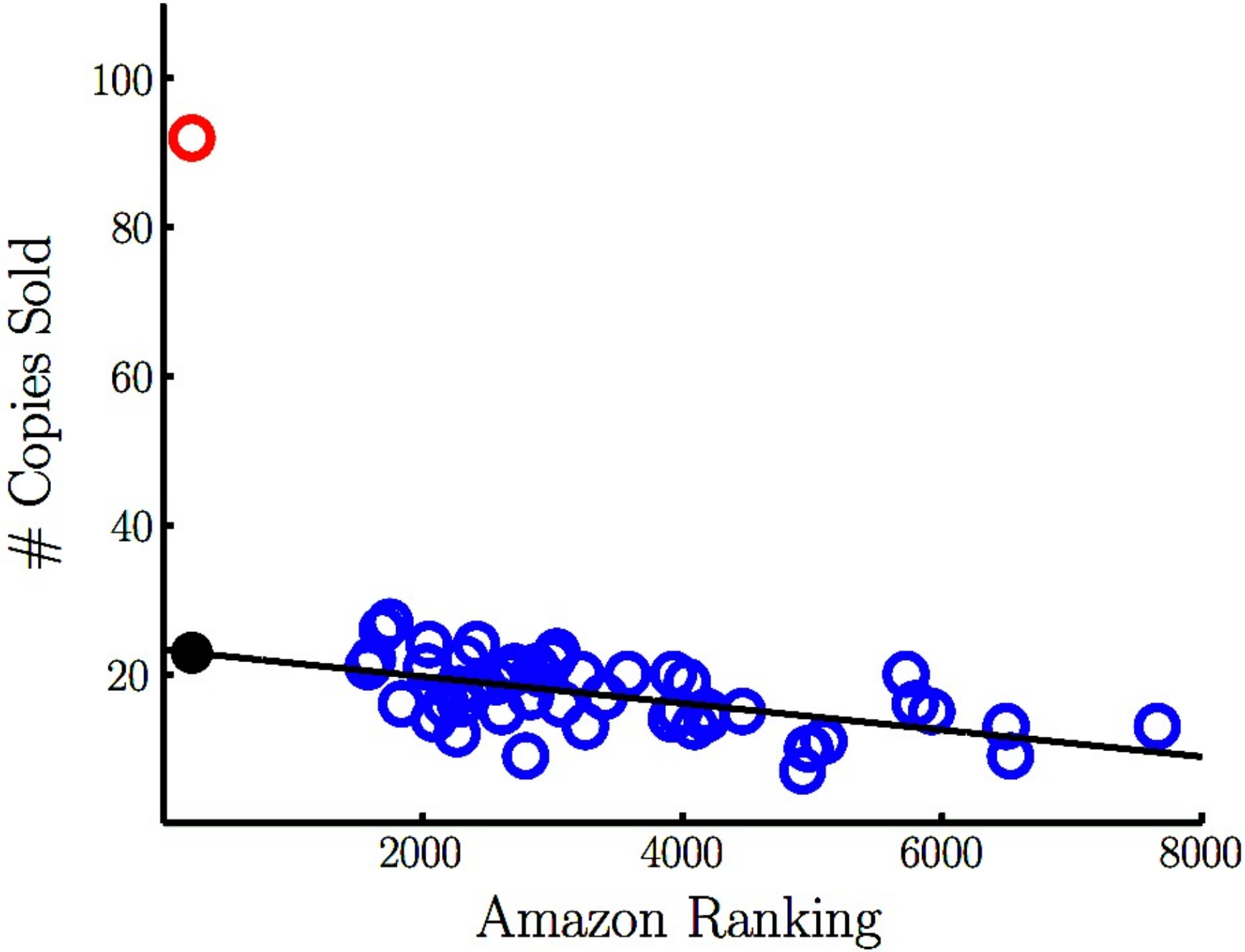
Make sure the training and test distributions are as close as possible…

- Example: importance weighting

Not always possible….

- If you don’t have access to some region of points in training, but they appear in the testing distribution


100
80
60
40
20
Copies Sold
2000
4000
6000
8000
Amazon Ranking


100
80
60
40
20
Copies Sold
2000
4000
6000
8000
Amazon Ranking

Credit card example

- Determine whether to approve credit cards given applicants' financial information
- Banks have lots of data:
  - Customer information
  - Whether they are good customers or not
- Are there any issues here?

age	32 years
gender	male
salary	40,000
debt	26,000
years in job	1 year
years at home	3 years
...	...

Approve for credit?

BUSINESS NEWS OCTOBER 9, 2018 / 10:12 PM / A YEAR AGO

Amazon scraps secret AI recruiting tool that showed bias against women

Jeffrey Dastin

8 MIN READ

The New York Times

Facial Recognition Is Accurate, if You're a White Guy

By Steve Lohr

Feb. 9, 2018

SONIA PAUL BACKCHANNEL 03.20.2017 12:00 AM

Voice Is the Next Big Platform, Unless You Have an Accent

It's super funny that Alexa can't understand my mom — until we need Alexa to use the web, drive a car, and do pretty much anything else.

We will spend 1~2 lectures towards the end of the semester to talk about various ethical considerations of ML.

Occam’s Razor

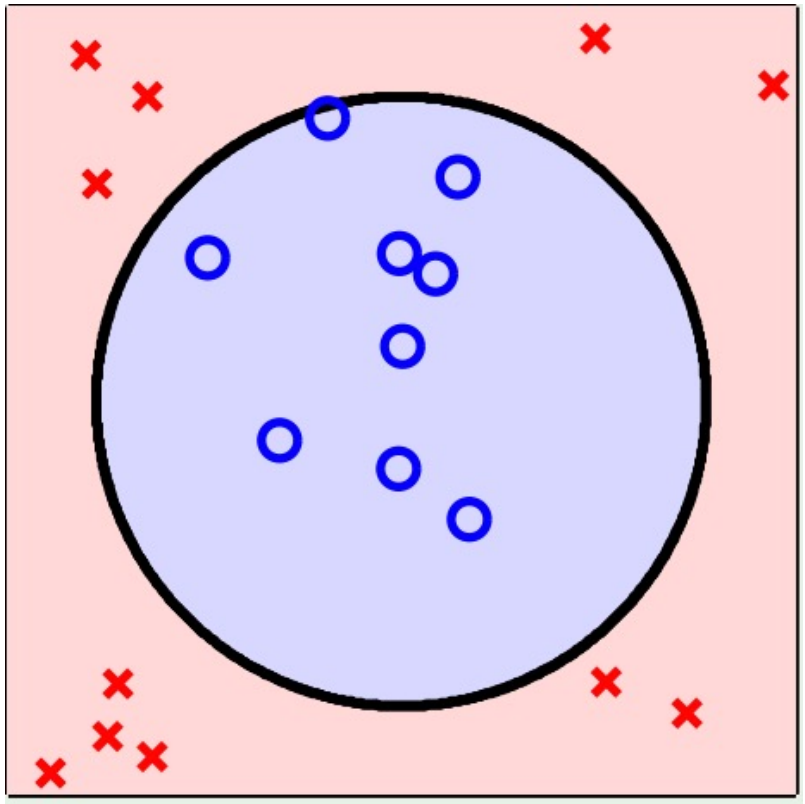
Sampling Bias

Data Snooping

Data Snooping

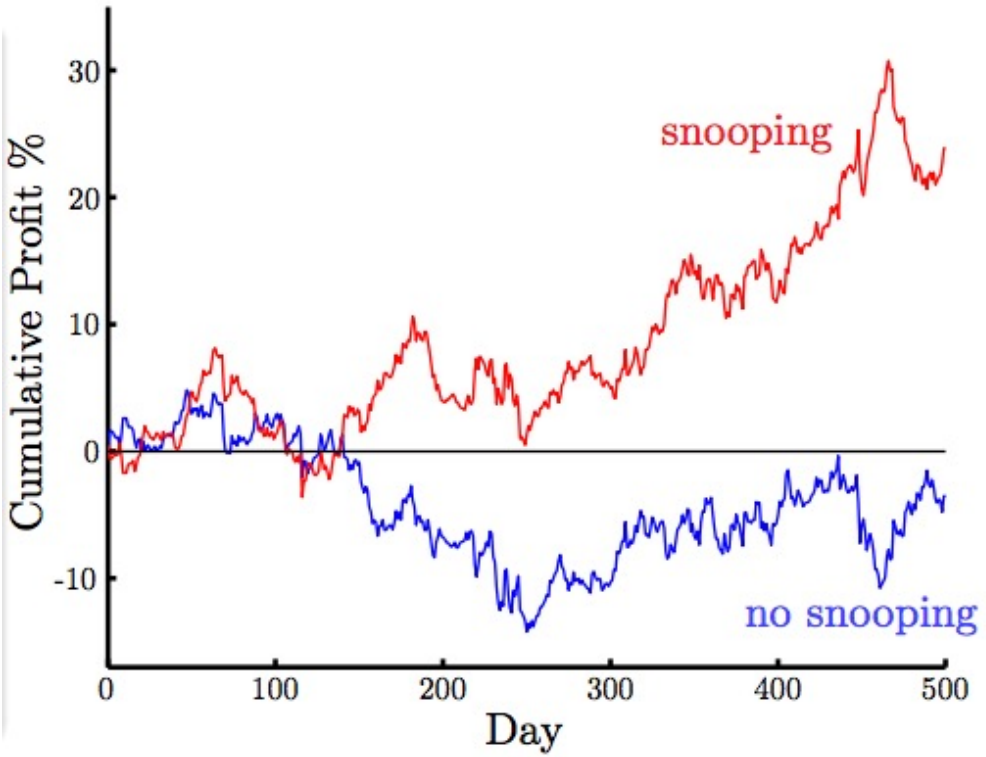
If a data set has affected any step in the learning process, its ability to assess the outcome has been compromised.

Shouldn’t looking at the data before selecting H



A Subtle Example

- Predict US Dollar vs. British Pound
  - $\vec{x}$: the change for the previous 20 days
  - y: the change in the 21th day
- Normalize data
- Randomly split D_{train} and D_{test}



- Where does snooping happen?
  - The normalization "looks at" D_{test}

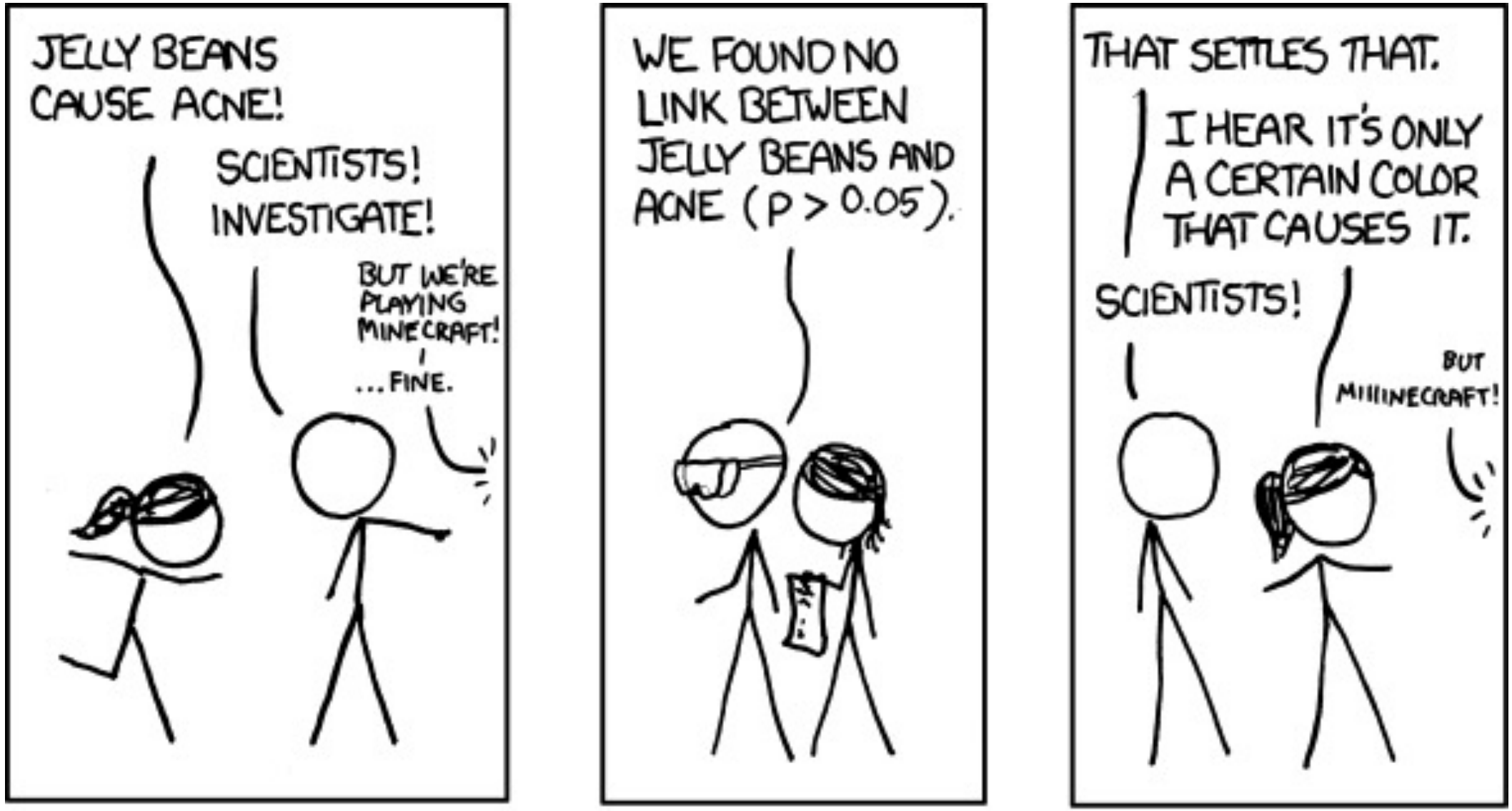
- How should you perform normalization in Q1 of HW2?

Reuse of a data set

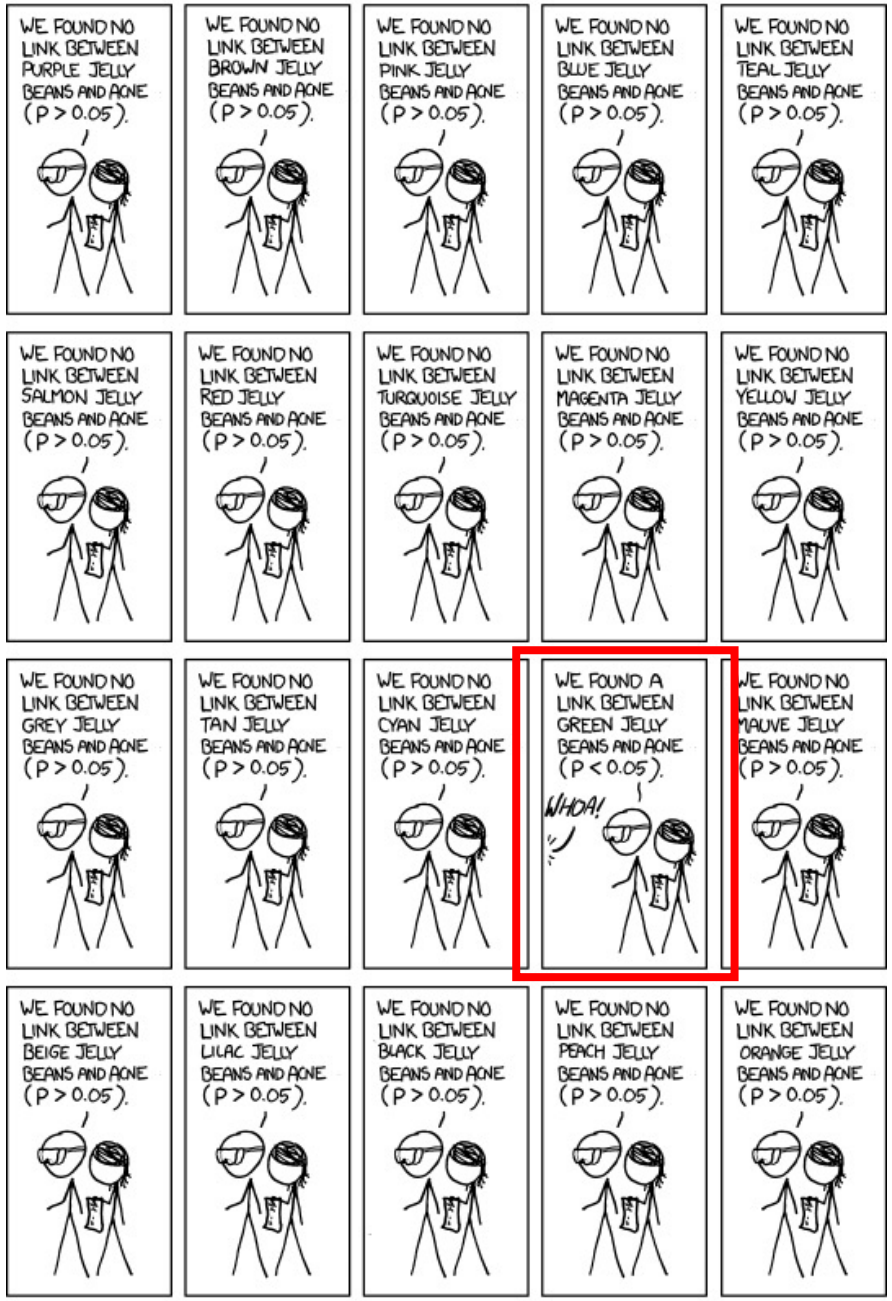
- Try one model after another **on the same data set**, you will eventually succeed.

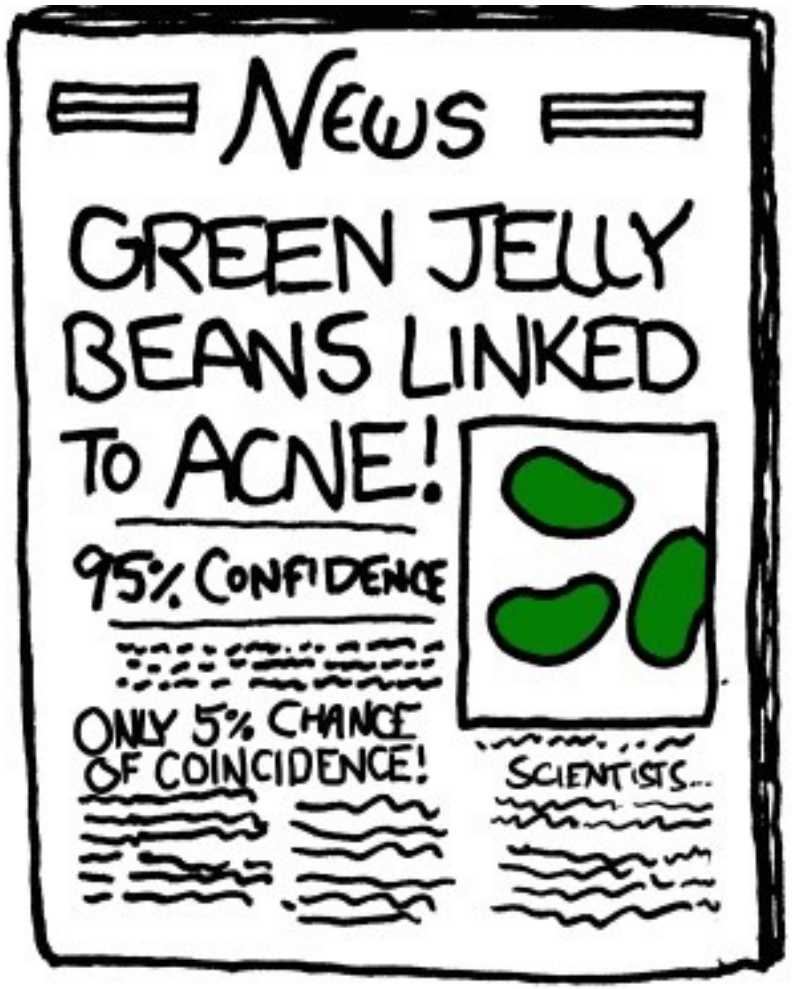
> "If you torture the data long enough, it will confess"

- VC dimension of the total learning models
- May even include what others tried (e.g., if you read their paper…)
- p-hacking…



From xkcd, by Randall Munroe: http://xkcd.com/882





From xkcd, by Randall Munroe: http://xkcd.com/882

What should we do…

Avoid data snooping

- Strict discipline
- E.g., be **honest** and lock the test data

Account for data snooping

- Measure how much data is contaminated
- E.g., what we discussed in validation

Occam’s Razor

Sampling Bias

Data Snooping

Course Plan

- Foundations
  - What's machine learning
  - Feasibility of learning
  - Generalization
  - Linear models
  - Non-linear transformations
  - Overfitting and how to avoid it
    - Regularization
    - Validation
- Techniques
  - Decision tree
  - Ensemble learning
    - Bagging and random forest
    - Boosting and Adaboost
  - Nearest neighbors
  - Support vector machine
  - Neural networks
  - …