Modes of learning + Model selection

CPSC 532S: Modern Statistical Learning Theory
9 February 2022
cs.ubc.ca/~dsuth/532S/22/

Admin

- Hybrid mode starts next week, in DMP 101
- Office hours still online-only this week

- A2 is up, due next Friday night
  - Groups of up to three, allowed separate per question
  - If you don’t have a group and want one, post on Piazza

- A1 grading: hopefully done this week

An analogy about MDL

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This includes any language with commands that "do whatever I choose them to do". Claiming that your answer is written in "MyOwnLanguage", where the command `x` means "read a sequence of numbers, split them into groups of three, and print the last numbers of those groups where the second number is less than the first", was clever the first time it was done. That was a *long* time ago.

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- **H**: Print "hello, world"
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Kolmogorov complexity

From Wikipedia, the free encyclopedia

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$x \in S|_x$, return mode $\{y_i : x = x_i\}$

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- **Even so**, can be interesting to compare $n_{\mathscr{H}}^{CON}$ for different sub-classes of $\mathscr{D}$

Is memorizing your lunch enough?

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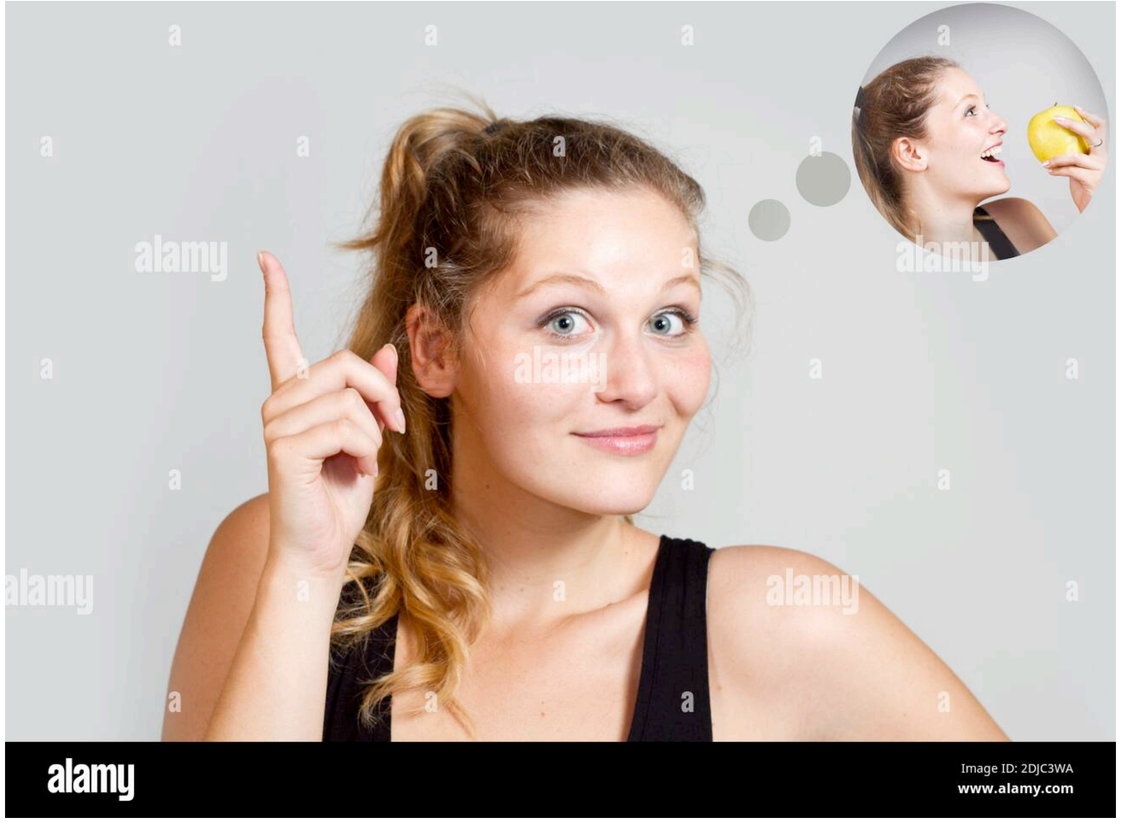

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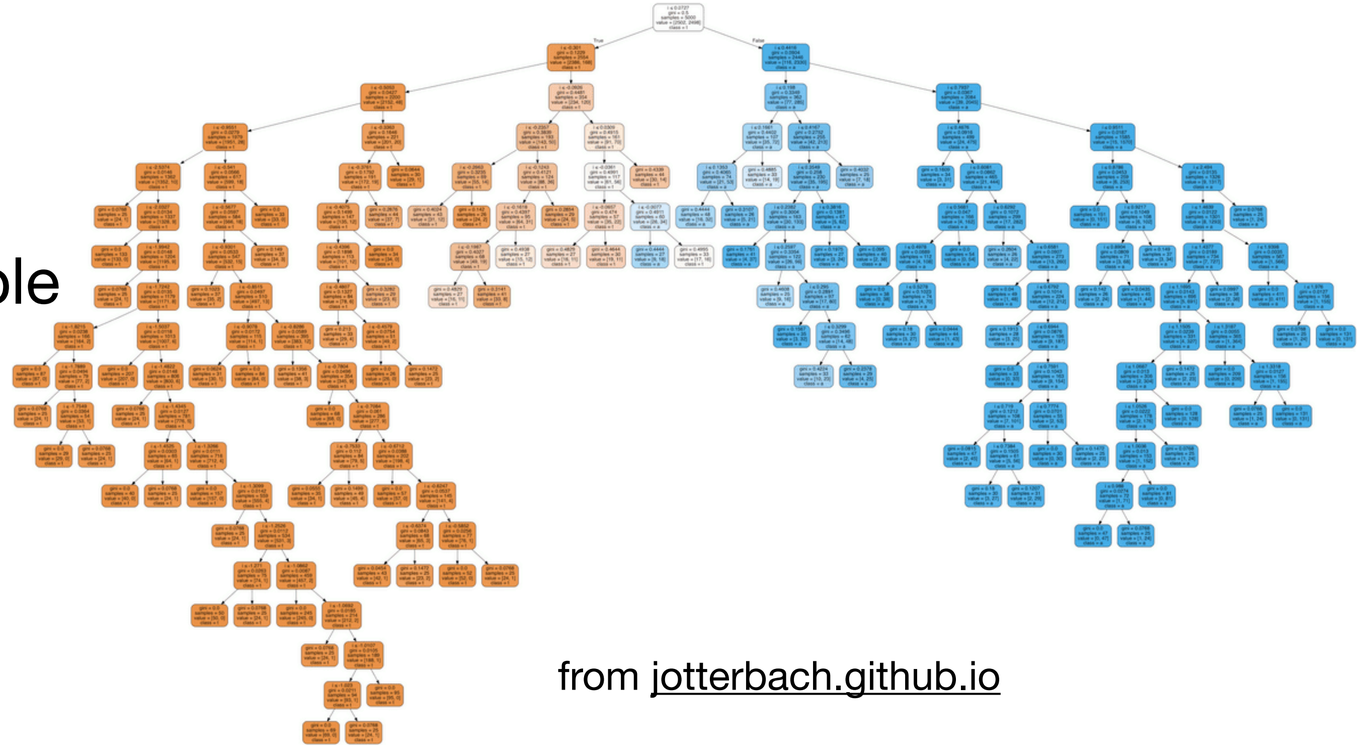
- Lots of work (unlike SSBD) ask about learning *given some assumptions on* $\mathscr{D}$
  - Of SSBD's models of learning, only consistency really allows this

(pause)

Model selection in practice

- Say we want to fit a decision tree,
  and are not sure how deep we should let it be
- Last time: pick $\mathscr{H}_k$ as depth-k trees, run SRM
  - But still need to pick weights…
  - MDL is one way
  - Not always best
  - Bounds can be conservative
  - Not always computationally feasible

- What if we want to fit
  either a decision tree
  or a linear classifier
  or a neural network
  or…?



from jotterbach.github.io

The CPSC 340 solution (i.e., what people actually do)

Validation Error

- How do we decide decision tree depth?
- We care about test error.
- But we can't look at test data.
- So what do we do?????

- One answer: Use part of the training data to approximate test error.
- Split training examples into training set and validation set:
  - Train model based on the training data. $L_S(h)$
  - Test model based on the validation data. $L_V(h)$

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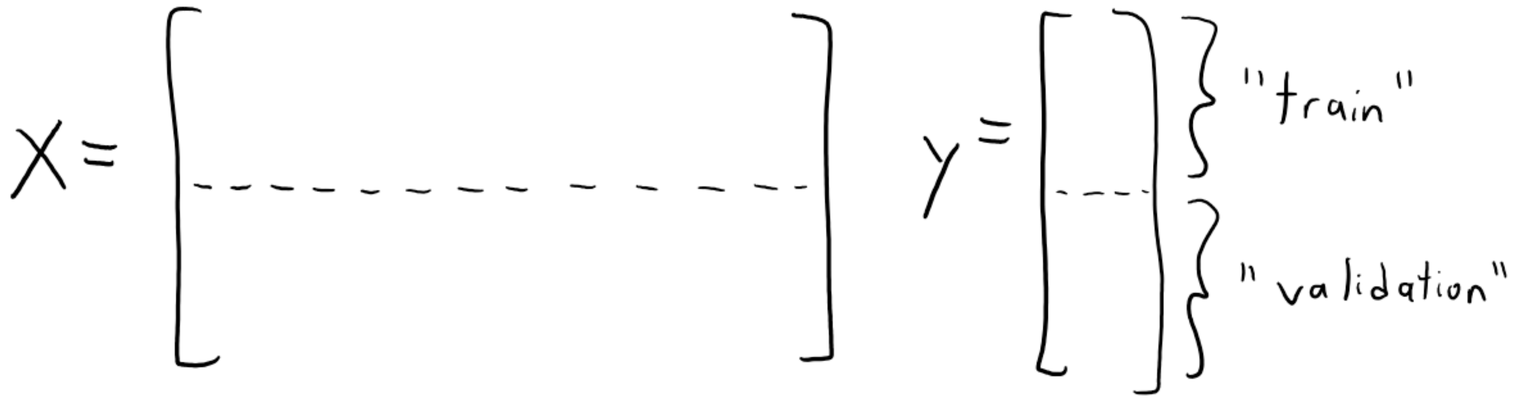

Step 1 is training: model = train(X_{train}, y_{train}) e.g. $\text{argmin}_h L_S(h)$

Step 2 is predicting: $\hat{y}$ = predict(model, $X_{validate}$)

Step 3 is validating: error = sum($\hat{y} \neq y_{validate}$) $L_V(h)$

Note: if examples are ordered, split should be random.

$\mathcal{H} = \mathcal{H}_1 \cup \mathcal{H}_2 \cup \mathcal{H}_3 \cup \ldots$

The CPSC 340 solution (i.e., what people actually do)

Notation: Parameters and Hyper-Parameters

- The decision tree rule values are called "parameters".
  - Parameters control how well we fit a dataset.
  - We "train" a model by trying to find the best parameters on training data.

- The decision tree depth is a called a "hyper-parameter".
  - Hyper-parameters control how complex our model is.
  - We can't "train" a hyper-parameter.
    - You can always fit training data better by making the model more complicated.
  - We "validate" a hyper-parameter using a validation score.

- ("Hyper-parameter" is sometimes used for parameters "not fit with data".)

The CPSC 340 solution (i.e., what people actually do)

Choosing Hyper-Parameters with Validation Set

- So to choose a good value of depth ("hyper-parameter"), we could:
  - Try a depth-1 decision tree, compute validation error. $\hat{h}_1 = \text{ERM}_{\mathcal{H}_1}(S)$
  - Try a depth-2 decision tree, compute validation error. $\hat{h}_2 = \text{ERM}_{\mathcal{H}_2}(S)$
  - Try a depth-3 decision tree, compute validation error. $\hat{h}_3 = \text{ERM}_{\mathcal{H}_3}(S)$
  - …
  - Try a depth-20 decision tree, compute validation error. $\hat{h}_{20} = \text{ERM}_{\mathcal{H}_{20}}(S)$
  - Return the depth with the lowest validation error.

$$k = \text{argmin}_k \, L_V(\hat{h}_k)$$

- After you choose the hyper-parameter, we usually re-train on the full training set with the chosen hyper-parameter. $\hat{h} = \text{ERM}_{\mathcal{H}_k}(S \cup V)$

or just take $\text{argmin}_k \, \hat{h}_k$

The CPSC 340 solution (i.e., what people actually do)

Digression: Optimization Bias

- Another name for overfitting is "optimization bias":
  - How biased is an "error" that we optimized over many possibilities?

- Optimization bias of parameter learning: (all of $\mathscr{H}$)
  - During learning, we could search over tons of different decision trees.
  - So we can get "lucky" and find one with low training error by chance.
    - "Overfitting of the training error".

- Optimization bias of hyper-parameter tuning: just $\{\hat{h}_1, \hat{h}_2, \ldots, \hat{h}_{20}\}$
  - Here, we might optimize the validation error over 20 values of "depth".
  - One of the 20 trees might have low validation error by chance.
    - "Overfitting of the validation error".

The CPSC 340 solution (i.e., what people actually do)

Digression: Example of Optimization Bias

- Consider a multiple-choice (a,b,c,d) "test" with 10 questions:
  - If you choose answers randomly, expected grade is 25% (no bias).
  - If you fill out two tests randomly and pick the best, expected grade is 33%.
    - Optimization bias of ~8%.
  - If you take the best among 10 random tests, expected grade is ~47%.
  - If you take the best among 100, expected grade is ~62%.
  - If you take the best among 1,000, expected grade is ~73%.
  - If you take the best among 10,000, expected grade is ~82%.
    - You have so many "chances" that you expect to do well.
- But on new questions the "random choice" accuracy is still 25%.

$\inf_{h \in \mathcal{H}} L_S(h)$ shrinks with $\mathcal{H}$

here $L_{\mathcal{D}}(h)$ is constant

so $\sup L_{\mathcal{D}}(h) - L_S(h)$ grows

The CPSC 340 solution (i.e., what people actually do)

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).

The CPSC 340 thought process

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.

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.

Hold-out set accuracy, quantitatively

- If V is independent of choosing h, for loss in $[0,B]$, immediately have

$$\left| L_V(h) - L_{\mathscr{D}}(h) \right| \leq B\sqrt{\frac{1}{2|V|}\log\frac{2}{\delta}}$$

  - No dependence on $\mathscr{H}$, A, etc; doesn't matter how we picked h

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- Find $\hat{\mathscr{H}} = \{\hat{h}_1, \ldots, \hat{h}_{|\hat{\mathscr{H}}|}\}$ based on a set S. For an independent V,

$$\left| L_V(h) - L_{\mathscr{D}}(h) \right| \leq B\sqrt{\frac{1}{2|V|}\log\frac{2|\hat{\mathscr{H}}|}{\delta}}$$

sup
$h \in \hat{\mathscr{H}}$

Validation set vs SRM

- Say we have $|S| = n$ and $|V| = m$
- Decompose $\mathscr{H}$ into $\mathscr{H}_1 \cup \mathscr{H}_2 \cup \cdots$; consider SRM with weights $6/(\pi^2 k^2)$
- $\text{Val}(S, V)$ takes $\text{argmin}_{h \in \{\text{ERM}_{\mathscr{H}_k}(S)\}} L_V(h)$

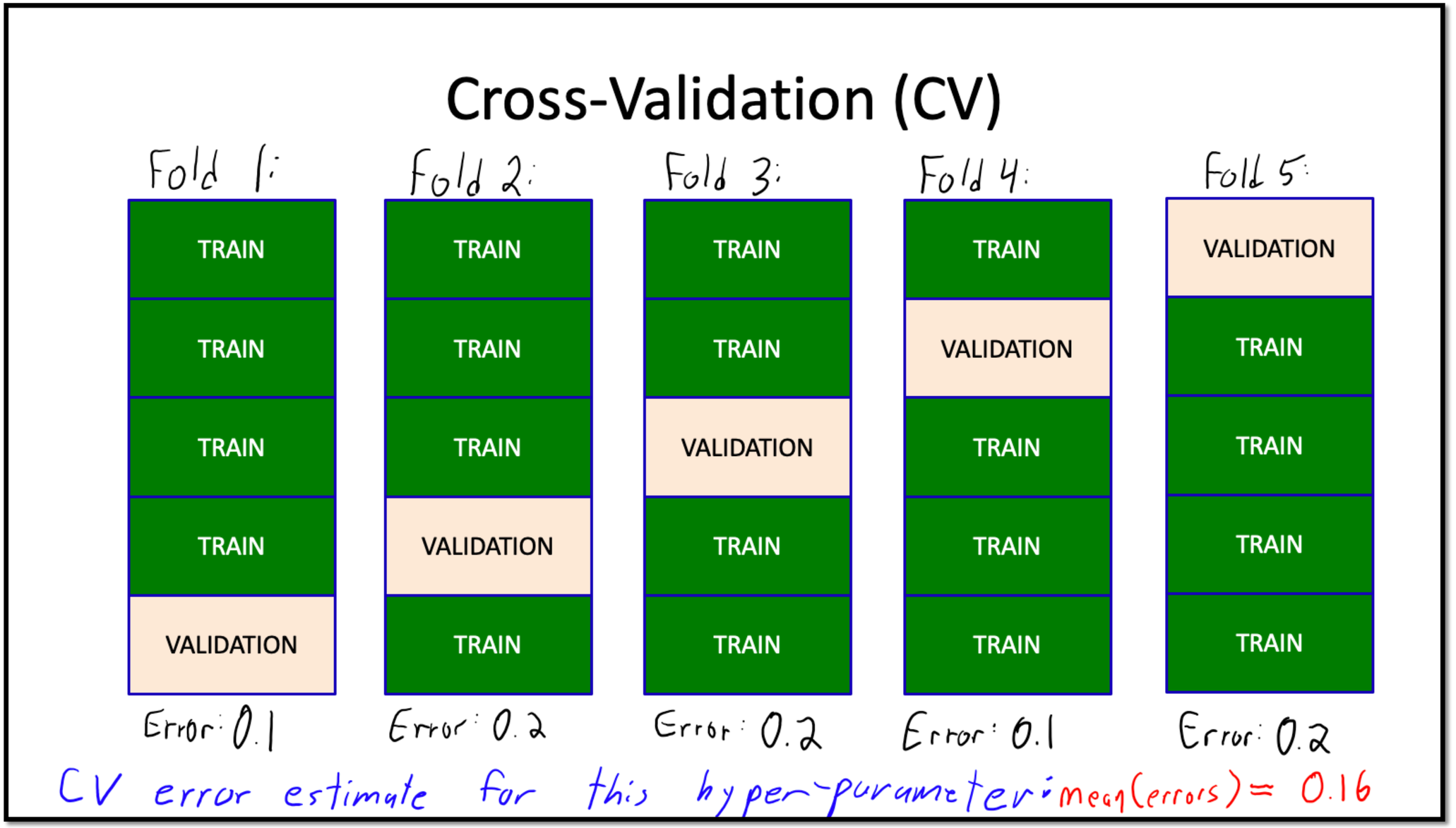
- Can show (MRT prop 4.3: union bound + Hoeffding) that

$$\left| L_{\mathscr{D}}(\text{ERM}_{\mathscr{H}_k}(S)) - L_V(\text{ERM}_{\mathscr{H}_k}(S)) \right| \leq \sqrt{\frac{1}{2m} \log \frac{4}{\delta}} + \sqrt{\frac{1}{m} \log k}$$

- Implies (MRT thm 4.4)

$$L_{\mathscr{D}}(\text{Val}(S, V)) - L_{\mathscr{D}}(\text{SRM}(S)) \leq 2\sqrt{\frac{1}{m} \log \max(k_{\text{Val}(S,V)}, k_{\text{SRM}(S)})} + 2\sqrt{\frac{1}{2m} \log \frac{4}{\delta}}$$

  - i.e. not too much worse than SRM with *part* of the data



We'll come back to analyze cross-validation soon (based on *stability* analyses)

Summary

- Models of learnability
  - Realizable PAC, Agnostic PAC
  - Nonuniform learning
  - Consistency
    - Silly to talk about whether consistent or not,
      but comparing sample complexities makes sense

- Picking models in practice
  - Validation sets
  - Simple bounds based on how many times you look at the val set
    - Hoeffding + union bound
  - Can prove: not too much worse than SRM (which ignores the val set)
  - More practical than SRM, usually

Massart's lemma: for $\mathcal{A} \subset \mathbb{R}^n$, if $\max_{a \in \mathcal{A}} \|a\| \le r$, $\quad \mathbb{E}_\sigma\left[\max_{a \in \mathcal{A}} \frac{1}{n} \boldsymbol{\sigma}^\top a\right] \le \frac{1}{n} r \sqrt{2 \log |\mathcal{A}|}$

$$\exp\left(\lambda \, \mathbb{E}_\sigma \max_a \sigma^\top a\right) \le \mathbb{E}_\sigma \exp\left(\lambda \max_a \sigma^\top a\right)$$

$$= \mathbb{E}_\sigma \max_a \exp(\lambda \, \sigma^\top a) \qquad \leftarrow \text{all} \ge 0$$

$$\le \mathbb{E}_\sigma \sum_a \exp(\lambda \, \sigma^\top a)$$

$$= \sum_a \mathbb{E}_\sigma \exp\left(\lambda \textstyle\sum_i \sigma_i a_i\right)$$

$$= \sum_a \mathbb{E}_\sigma \prod_{i=1}^n \exp(\lambda \sigma_i a_i)$$

$$= \sum_a \prod_i \frac{1}{2}\left(e^{\lambda a_i} + e^{-\lambda a_i}\right)$$

$$\le \sum_a \prod_i e^{\lambda^2 a_i^2/2}$$

$$= \sum_a e^{\lambda^2 \|a\|^2/2}$$

$$\le \sum_a e^{\lambda^2 r^2/2} = |\mathcal{A}| \, e^{\lambda^2 r^2/2}$$

$\mathcal{H}_S = \{(h(z_1), \ldots, h(z_n)) : h \in \mathcal{H}\} \subseteq \mathbb{R}^n$

$\hat{\mathcal{R}}_S(\mathcal{H}) = \mathbb{E}_\sigma \max_{h_S \in \mathcal{H}_S} \frac{1}{n} \sigma^\top h_S$

$\max\{1, 2, 0.5, 3\} \ll 1 + 2 + 0.5 + 3$

but $\max\{1, 2, 1000, 3\} \approx 1 + 20 + 1000 + 2$

$$\frac{e^x + e^{-x}}{2} \le e^{\frac{1}{2}x^2}$$

$$\le \left(\frac{1}{\sqrt{2}} + \frac{\sqrt{2}}{2}\right) r \sqrt{\log |\mathcal{A}|}$$

done!

$$\therefore \mathbb{E}_\sigma \max_a \sigma^\top a \le \frac{1}{\lambda} \log |\mathcal{A}| + \lambda \frac{r^2}{2}$$

$$\mathbb{E}_\sigma \max_a \sigma^\top a \le \inf_{\lambda > 0} \frac{1}{\lambda} \log |\mathcal{A}| + \lambda \frac{r^2}{2}$$

$$\log |\mathcal{A}| = \frac{r^2}{2} \lambda^2$$

$$\lambda = \frac{1}{r} \sqrt{2 \log |\mathcal{A}|}$$