Model Selection, Validation, and Regularization

Lecture 10

Last Time

- The ***no-free-lunch theorem*** tells us that there is no universal learning algorithm that will work best on all problems.

- Further, for every algorithm, there is a problem it fails on, even though another succeeds

- Instead, for every learning problem we must balance the bias-complexity tradeoff using prior knowledge

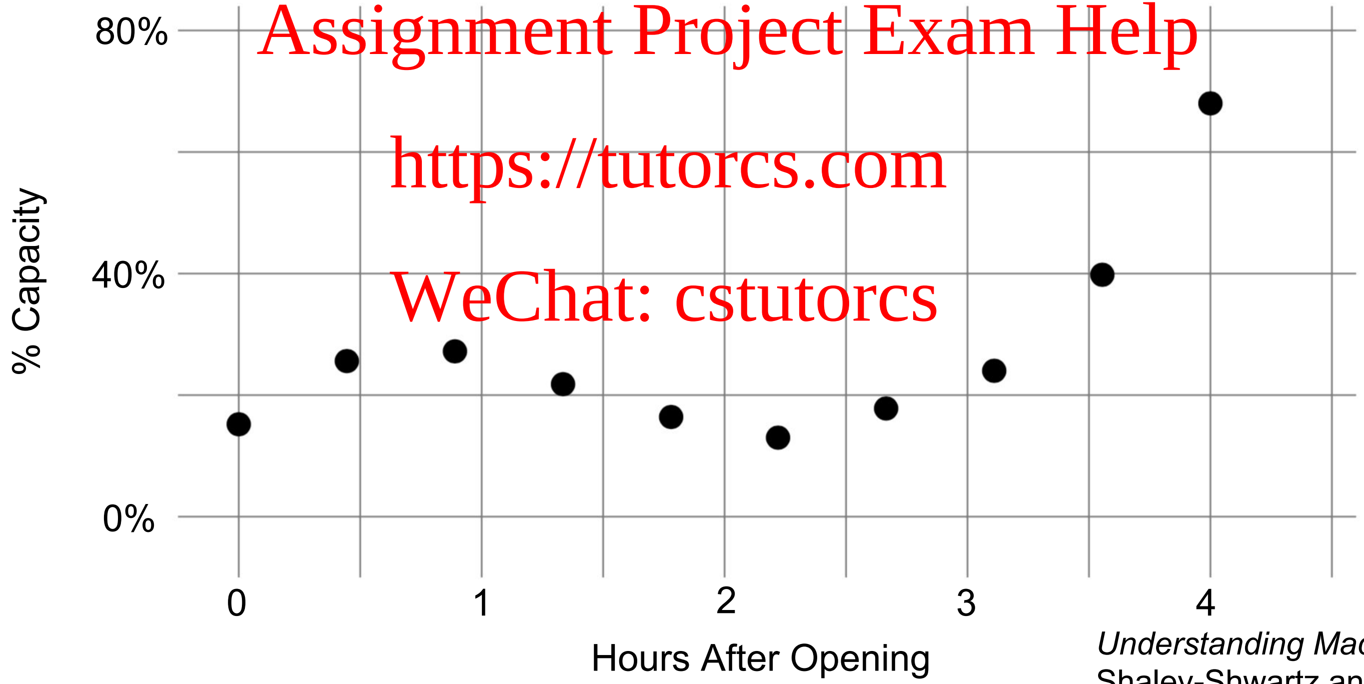
- Textbook: chapter 5

This Class

- How do we balance the bias-complexity tradeoff in practice?
- Textbook: chapters 11.0, 11.2, 11.3, 13.0, 13.1, 13.4

Motivating Example

Let's determine the popularity of Jo's as a function of time:



Understanding Machine Learning. Shalev-Shwartz and Ben-David, 2014.

Let’s Model It

Polynomial regression of varying degrees:

Which one would you choose and why?

Understanding Machine Learning.
Shalev-Shwartz and Ben-David, 2014.

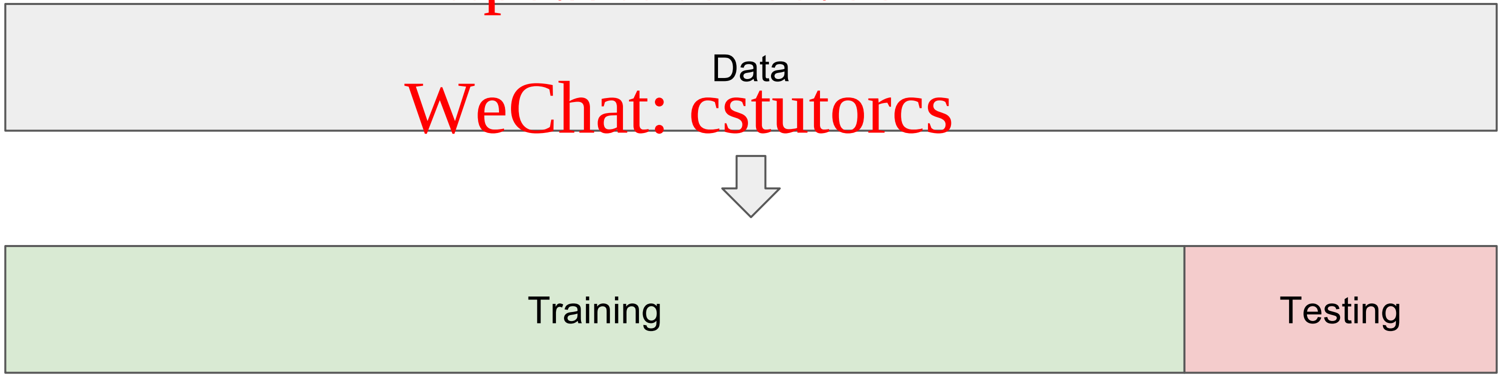
Model Selection and Validation

The Need for Validation

- As we increase polynomial order, we lower empirical risk
- But seems like overfitting!
- Q: How do we formalize this intuition and apply it to high-dimensional data?
- A: Find balance between approximation and estimation errors via validation

Previous Set Up

So far we've held out a test set to get an unbiased estimate of $L_{\mathcal{D}}(h)$

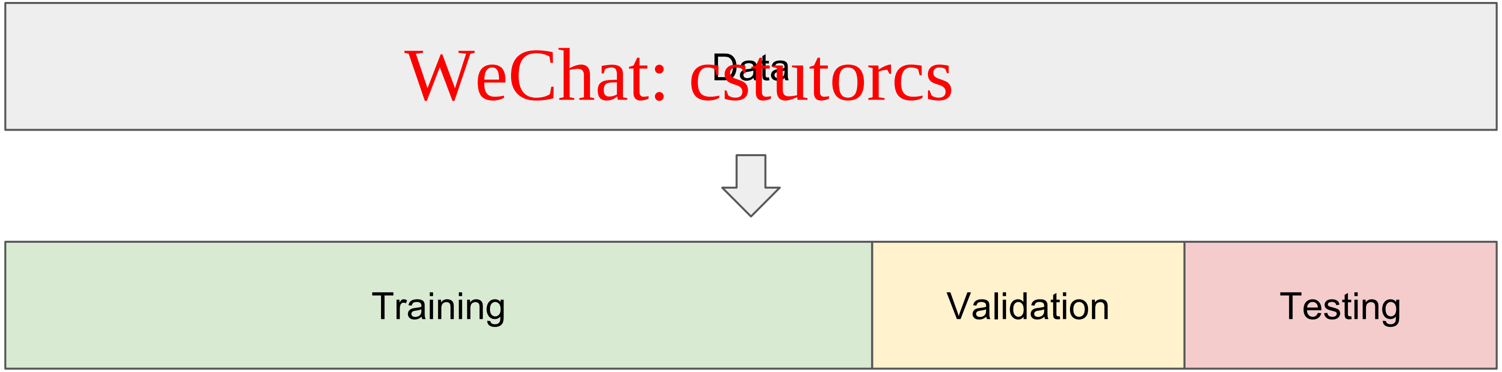


No Peeking!

- If we evaluate multiple hypotheses on the test set, and then pick the best one, then it is no longer an unbiased estimate of $L_{\mathcal{D}}(h)$

Training-Validation-Test Split

Use training data to train, validation data to select the best model, and testing data for a estimation of true error



Model Selection with Validation

- Train different algorithms (or the same algorithm with different hyperparameters) on a given training set

- Now, to choose a single hypothesis from H we choose the one that minimizes the error over the validation set

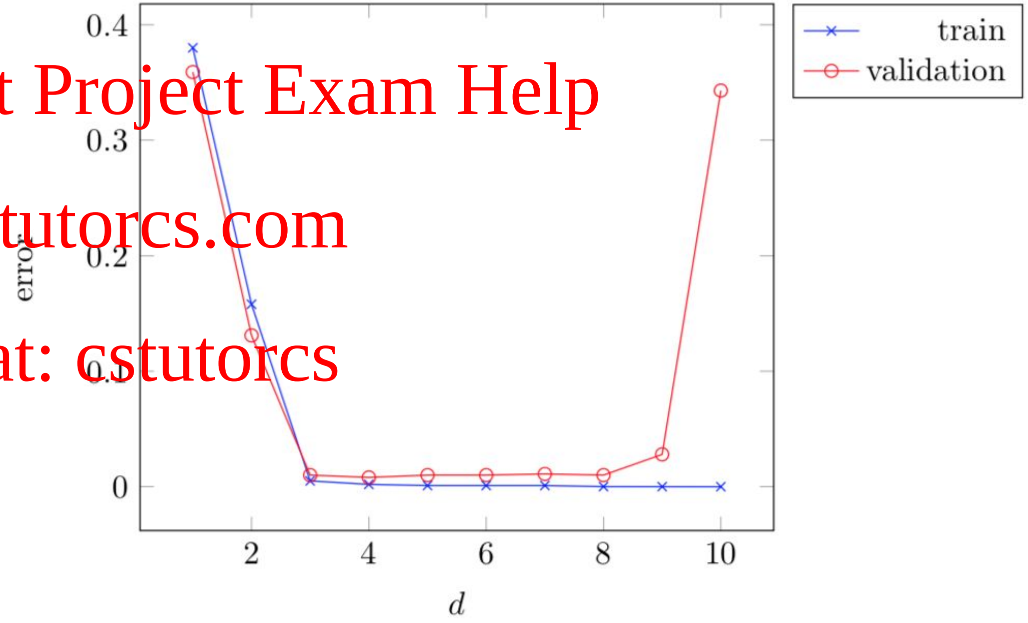
- Error on the validation set approximates the true error

Model Selection Curves

Shows Training and Validation error as a function of complexity

Recall Jo's Example:

- Training error decreases monotonically
- Validation decreases then increases (Overfitting)



Understanding Machine Learning. Shalev-Shwartz and Ben-David, 2014.

Bounding the Loss via Validation

Any hypothesis, maybe one from ERM

$\ell(h, (\mathbf{x}, y))$

THEOREM 11.1 *Let* $\boxed{h}$ *be some predictor and assume that the* $\boxed{\textit{loss function}}$ *is in* $[0,1]$. *Then, for every* $\delta \in (0,1)$, *with probability of at least* $1-\delta$ *over the choice of a validation set* V *of size* m_v *we have*

$$|\boxed{L_V(h)} - L_{\mathcal{D}}(h)| \;\leq\; \sqrt{\frac{\log(2/\delta)}{2\,m_v}}.$$

$$\frac{1}{m_v}\sum_{i=1}^{m_v} \ell(h, (\mathbf{x}_i^v, y_i^v))$$

Proof

- Recall Hoeffding's Inequality: $\mathbb{P}\left[\left|\frac{1}{m}\sum_{i=1}^{m}\theta - \mu\right| > \epsilon\right] \leq 2\exp\left(\frac{-2m\epsilon^2}{(b-a)^2}\right)$

- Define $\delta = 2\exp\left(-2m_v\epsilon^2\right)$

- Solve for ϵ: $\epsilon = \sqrt{\frac{\log(2/\delta)}{2m_v}}$

- Substitute ϵ and δ into Hoeffding's Inequality, where b = 1 and a = 0

Rearranging to Upper Bound on Loss

$$|L_V(h) - L_{\mathcal{D}}(h)| \leq \sqrt{\frac{\log(2/\delta)}{2m_v}}$$

implies

$$L_{\mathcal{D}}(h) \leq L_V(h) + \sqrt{\frac{\log(2/\delta)}{2m_v}}$$

Comparison with UC Upper Bound

Validation Upper Bound:

$$L_{\mathcal{D}}(h) \leq L_V(h) + \sqrt{\frac{\log(2/\delta)}{2m_v}}$$

Uniform Convergence Upper Bound

$$L_{\mathcal{D}}(h_S) \leq L_S(h_S) + \sqrt{\frac{\log|\mathcal{H}| + \log(2/\delta)}{2m}}$$

Question

What Went Wrong?

Steve plots a model selection curve for predicting the popularity of Andrew's. He considers polynomial regression with all maximum degrees 1 to 10 (inclusive). Using a validation set of size $m_v = 100$ he sees that degree 4 (h_4) has the best validation error of 0.1. Using the upper bound $L_{\mathcal{D}}(h) \leq L_V(h) + \sqrt{\frac{\log(2/\delta)}{2m_v}}$ he concludes that with probability ≥95%, $L_{\mathcal{D}}(h_4) \leq L_V(h_4) + \sqrt{\frac{\log(2/0.05)}{200}} \leq 0.24$. However, when he (somehow magically) evaluates $L_{\mathcal{D}}(h_4)$, it is 0.26. What went wrong?

A: Nothing, it happens with <5% chance

B: Wrong value for δ

C: He didn't meet the bound's assumptions

D: Wrong value for m_v

Answer

Answer: He didn't meet the bound's assumptions (C)

- Tricky mistake!

- He evaluated $L_V(h)$ for all ten hypotheses in $\mathcal{H}_S$ (best of each kind on S)

- Just like the bound on the empirical risk minimizer, we have to account for how many hypotheses we evaluated on the validation data to pick h:

$$L_{\mathcal{D}}(h) \leq L_V(h) + \sqrt{\frac{\log|\mathcal{H}_S| + \log(2/\delta)}{2m_v}}$$

k-fold Cross Validation

Previous methods work great when you have a ton of data
What if you don't want to "waste data" on those?

General idea of k-fold across all sets:

1. Split data into *k* subsets of equal size
2. For each fold, train on the union of all other folds and estimate error using the fold
3. Average the error across all folds

Iteration 1	Test	Train	Train	Train	Train
Iteration 2	Train	Test	Train	Train	Train
Iteration 3	Train	Train	Test	Train	Train
Iteration 4	Train	Train	Train	Test	Train
Iteration 5	Train	Train	Train	Train	Test

What if Learning Fails?

What if Learning Fails?

Plenty of options:

- Get a larger sample
- Change the hypothesis class by:
    - Enlarging it
    - Reducing it
    - Completely changing it
    - Changing the parameters you consider
- Change the feature representation of the data
- Change the optimization algorithm used to apply your learning rule

Need to smartly choose what is the issue: Approximation or Estimation error

Error Decomposition Using Validation

Using validation to see what is wrong (two types of error)

Recall:

$$\epsilon_{app} = \min_{h \in H} L_D(h)$$

$$\epsilon_{est} = L_D(h_S) - \epsilon_{app}$$

What do these depend on?

Types of Error and their Dependencies

Approximation Error Depends on:

- Underlying distribution *D*
- Hypothesis class *H*

Improving Approximation error:

- Increase size of *H* or change it
- Change featurization of data

Estimation error Depends on:

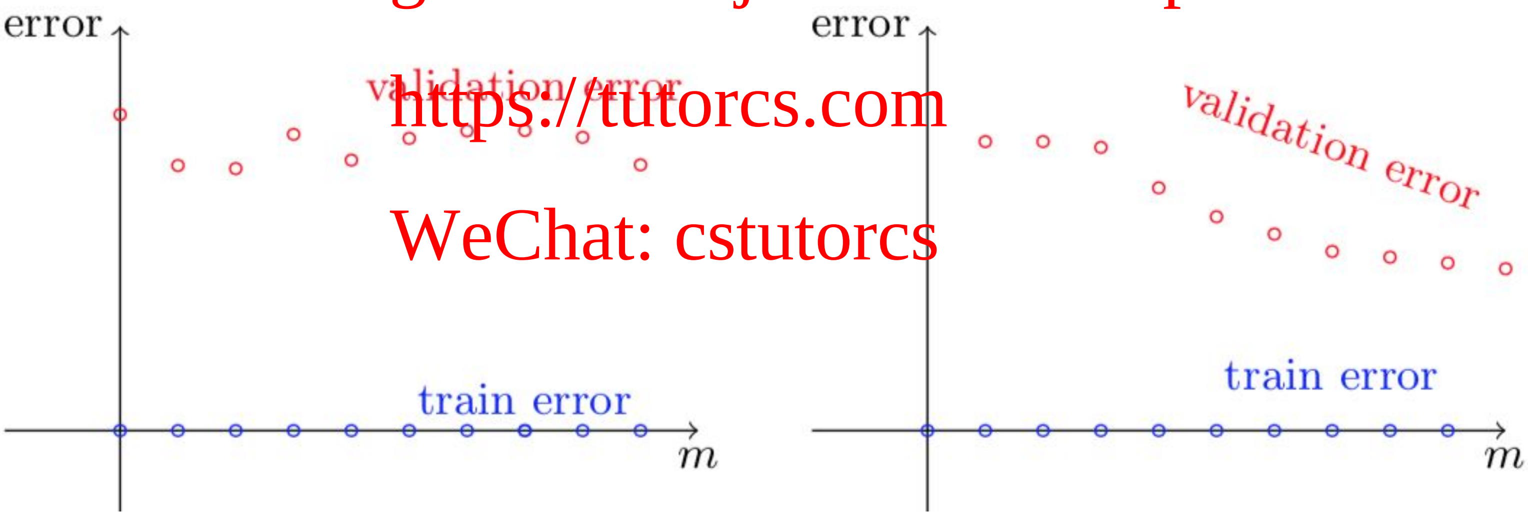
- Underlying distribution *D*
- Hypothesis class *H*
- Sample Size

Improving Estimation error:

- Obtain more training samples
- Reduce *H*

Learning Curves

Train the algorithm on prefixes of the data of increasing sizes, and plot:



Understanding Machine Learning.
Shalev-Shwartz and Ben-David, 2014.

Learning Curves

- If approximation error is greater than 0 expect training error to grow and validation error to decrease as sample size increases.

- If class is agnostic PAC learnable, they converge on the approximation error. This can be extrapolated from the curves as well.

Regularization

Fine-Tuning the Bias-Complexity Tradeoff

- Two types of error: approximation and estimation

- What tools do we have to adjust the spectrum?
  - Change the model, Change the representation

- What if we don't want to throw all of our hard work away? Can we keep our representation (training data and hypothesis class) and adjust the tradeoff?

Regularization

A regularizer balances between empirical risk and simpler hypotheses:

$$R : \mathbb{R}^d \to \mathbb{R}$$

Regularized Loss Minimization: Combines both empirical risk and regularizer minimization:

$$\underset{w}{\operatorname{argmin}}(L_S(w) + R(w))$$

Simple(?) Regularizer

$$h_w(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \dots + w_k x^k$$

$$R(w) = \lambda \max(\{k \quad \text{where } w_k \neq 0\})$$

In words? Advantages? Challenges?

Tikhonov Regularization

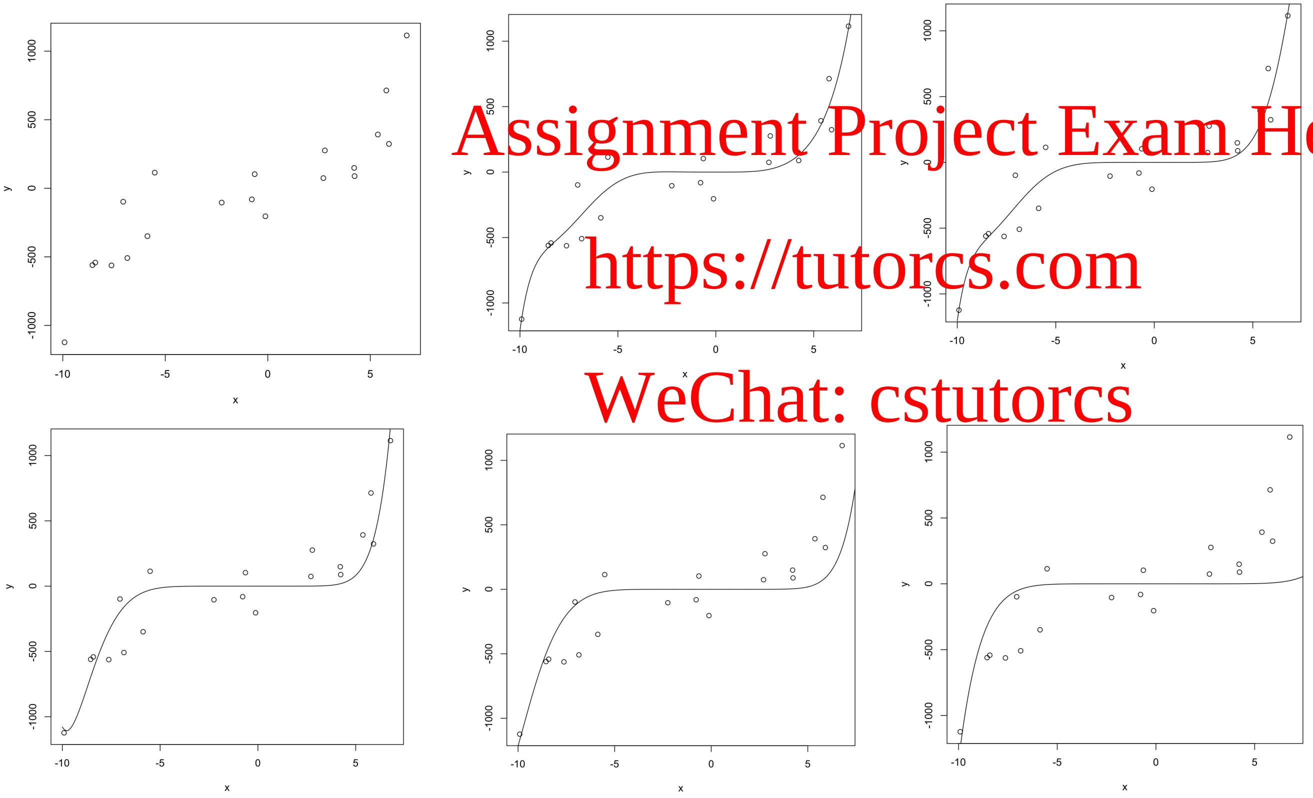
Also known as L2 regularization or weight decay

$$R(w) = \lambda ||w||_2^2 \qquad ||w||_2 = \sqrt{\sum_{i=1}^{d} w_i^2}$$

Ridge regression = linear/polynomial regression + Tikhonov regularization:

$$\underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} \left(\lambda ||\mathbf{w}||_2^2 + \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} (\langle \mathbf{w}, \mathbf{x}_i \rangle - y_i)^2 \right)$$

Ridge Regression Demo (degree=10)



Regularization λ

10^-5

10^-4

10^-3

10^-2

10^-1

10^2: flat

ERM for Ridge Regression

Gradient of the empirical risk is $(2\lambda mI + A)\mathbf{w} - \mathbf{b}$ where

$$A = \left(\sum_{i=1}^{m} \mathbf{x}_i \mathbf{x}_i^\top\right) \qquad \mathbf{b} = \sum_{i=1}^{m} y_i \mathbf{x}_i$$

Setting equal to 0 and solving for $\mathbf{w}$ gives

$$\mathbf{w} = (2\lambda mI + A)^{-1}\mathbf{b}$$

Tikhonov Regularization for other Models

- We can add Tikhonov regularization to any risk function
- Gradient is a linear operator so we just add the gradient of R to the usual one
- For example, to use Tikhonov regularization for multiclass logistic regression:

$$\frac{\partial L_S(h_{\mathbf{w}}) + R(h_{\mathbf{w}})}{\partial w_{st}} = \frac{1}{m}\sum_{i=1}^{m}(h_{\mathbf{w}}(\mathbf{x}_i)_s - \mathbf{1}[y_i = s])x_{it} + 2\lambda w_{st}$$

Review

- A held-out ***validation set*** is a critical tool for model selection

- It helps assess where on the bias-complexity tradeoff a hypothesis is

- ***Regularizers*** like Tikhonov regularization give us a knob λ to adjust bias-complexity tradeoff for a fixed hypothesis class

- Textbook: chapters 11.0, 11.2, 11.3, 13.0, 13.1, 13.4

Next Class

- Our final tool of learning theory: what makes a hypothesis class learnable? Can infinite hypothesis classes ever be learnable?
- Textbook: chapters 6, 9.1.3