Lecture 3:

Overview
Fall 2018

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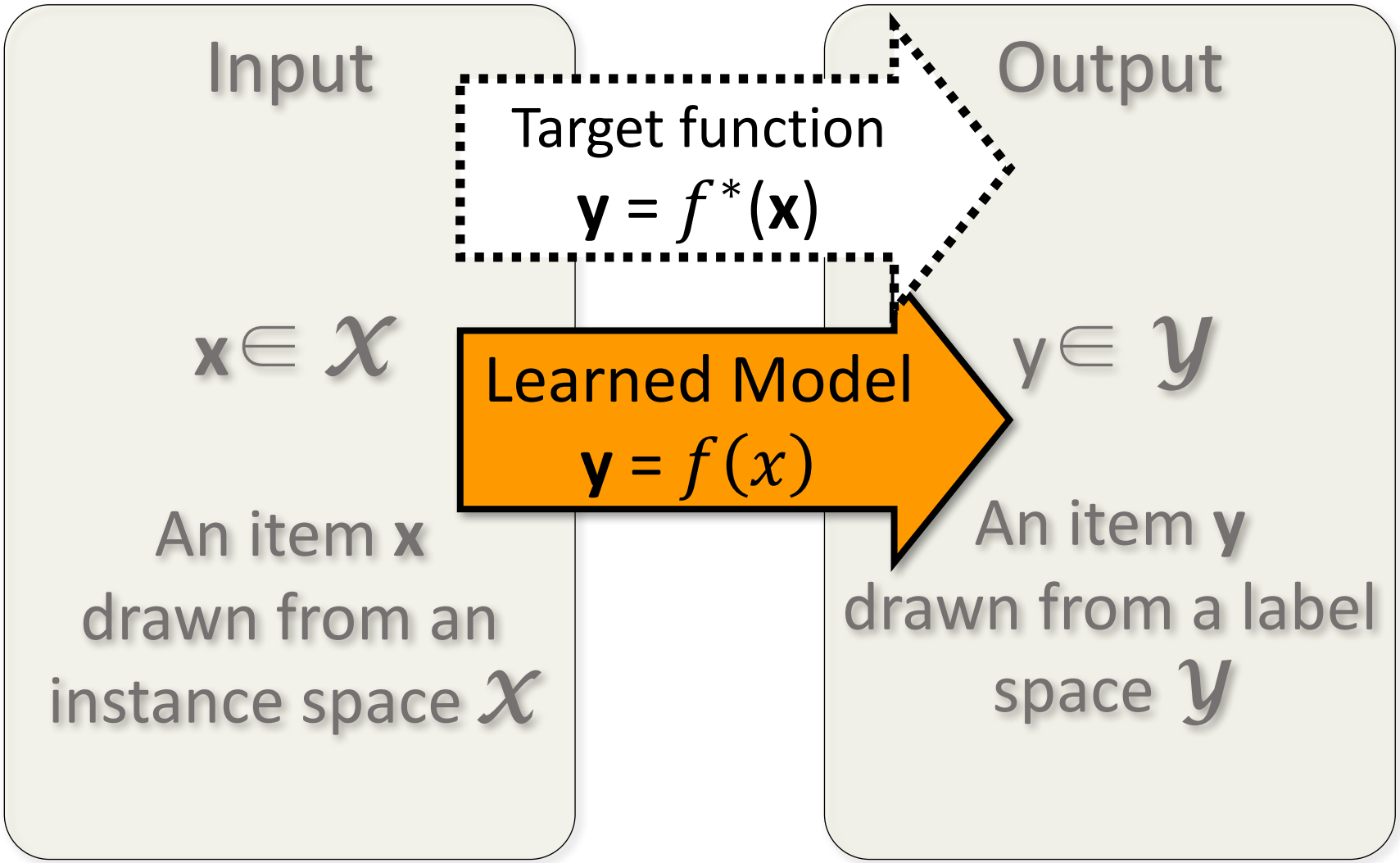
What is Learning

- The Badges Game……
  - This is an example of the key learning protocol: supervised learning
- Issues:
  - Prediction or Modeling?
  - Representation
  - Problem setting
  - Background Knowledge
  - When did learning take place?
  - Algorithm

Learning the mapping



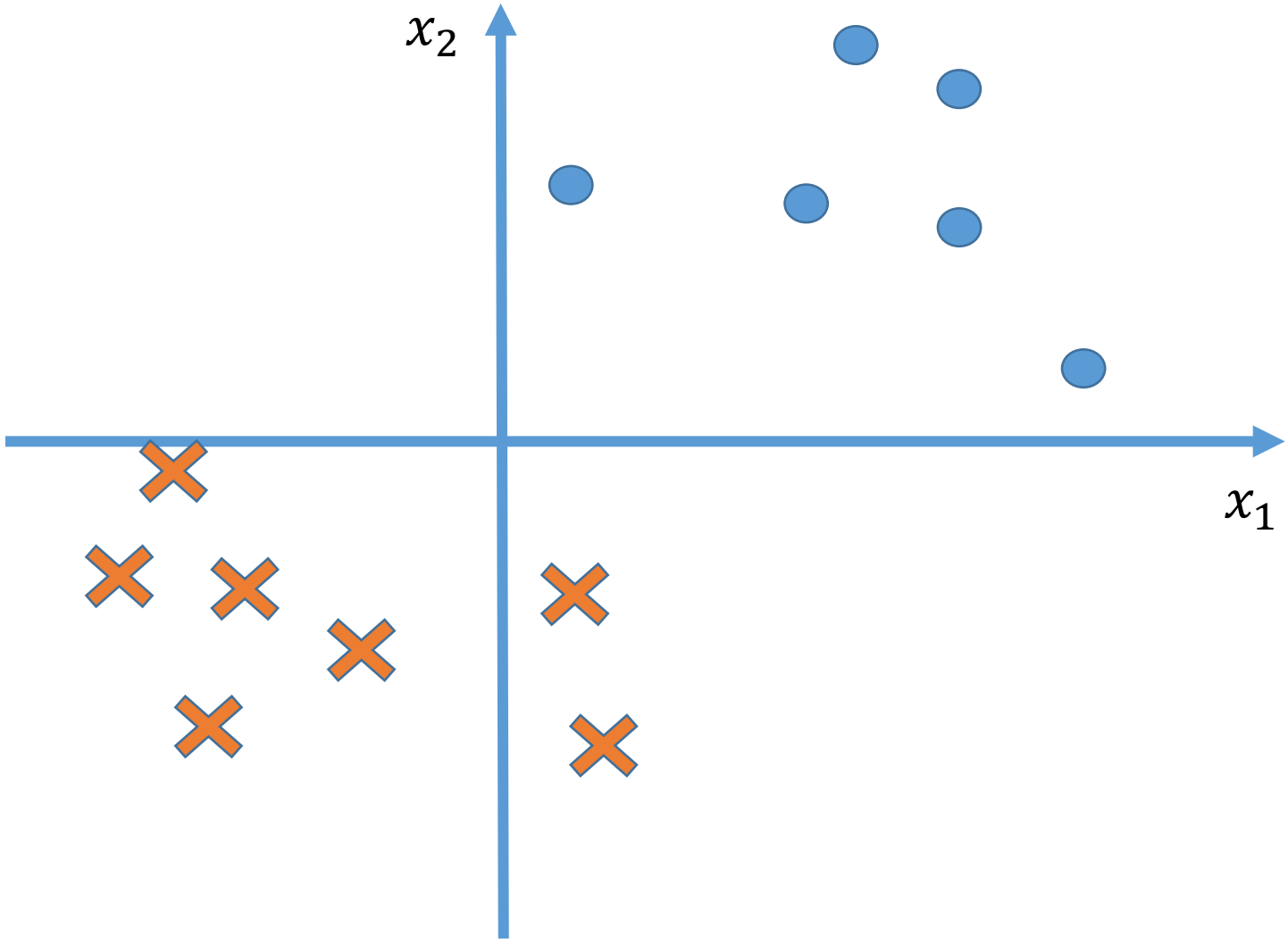
Using supervised learning

- What is our instance space?
  - Gloss: What kind of features are we using?
- What is our label space?
  - Gloss: What kind of learning task are we dealing with?
- What is our hypothesis space?
  - Gloss: What kind of functions (models) are we learning?
- What learning algorithm do we use?
  - Gloss: How do we learn the model from the labeled data?
- What is our loss function/evaluation metric?
  - Gloss: How do we measure success? What drives learning?

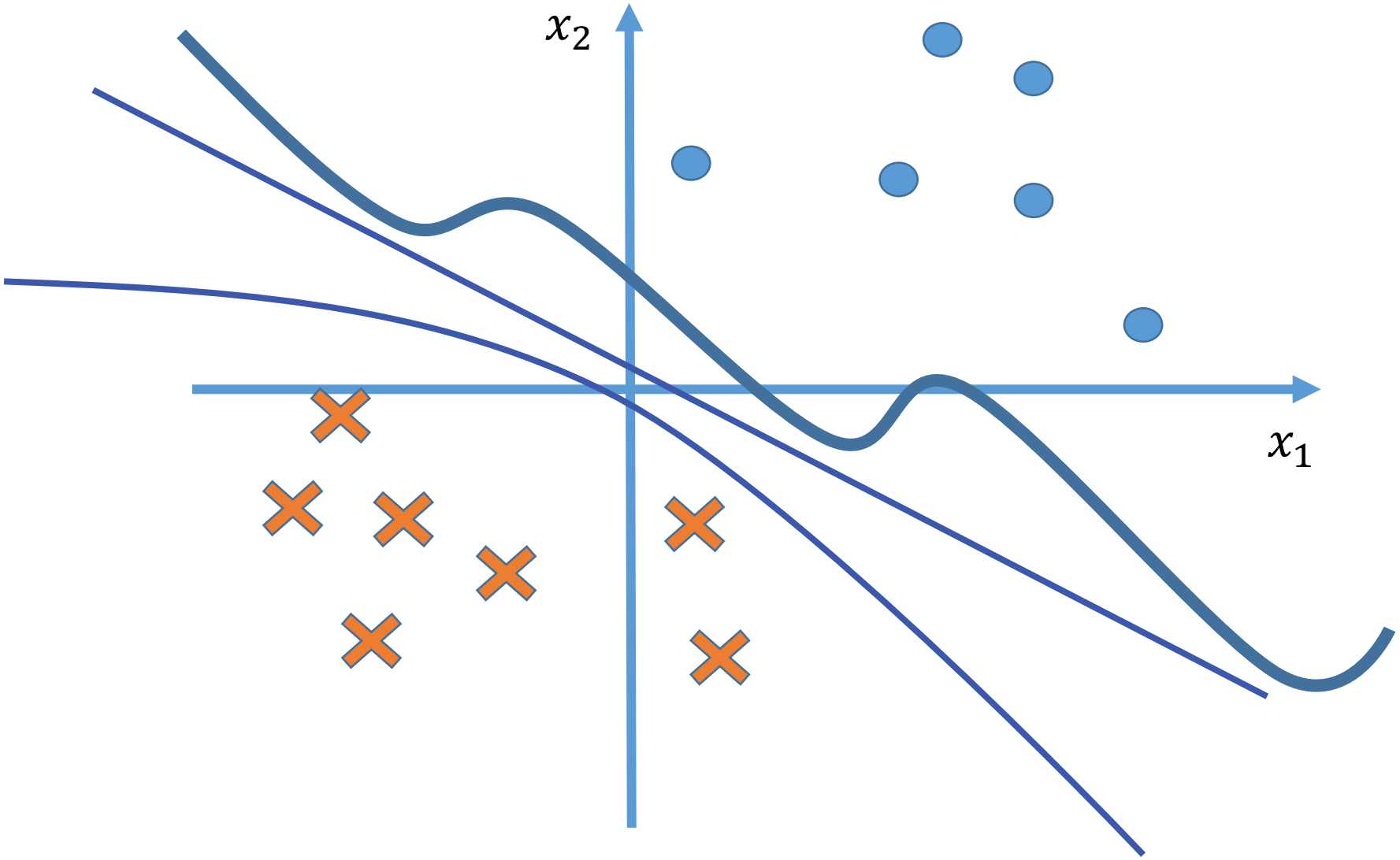
Views of Learning

- Learning is the removal of our remaining uncertainty:
  - Suppose we knew that the unknown function was an m-of-n Boolean function, then we could use the training data to infer which function it is.
- Learning requires guessing a good, small hypothesis class:
  - We can start with a very small class and enlarge it until it contains an hypothesis that fits the data.
- We could be wrong !
  - Our guess of the hypothesis space could be wrong
    - y=x4 Λ one-of (x1, x3) is also consistent

Example problem

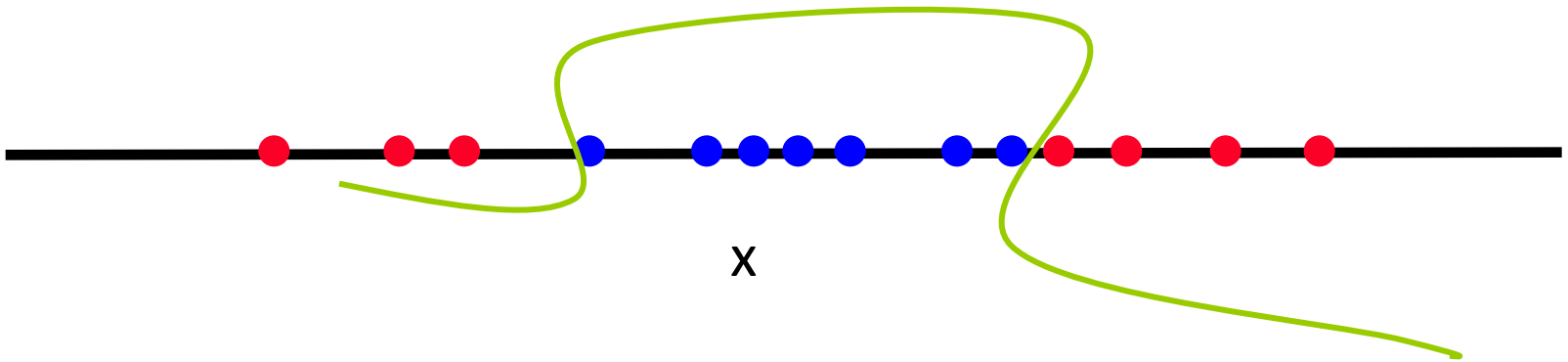


Hypothesis space:



Functions Can be Made Linear

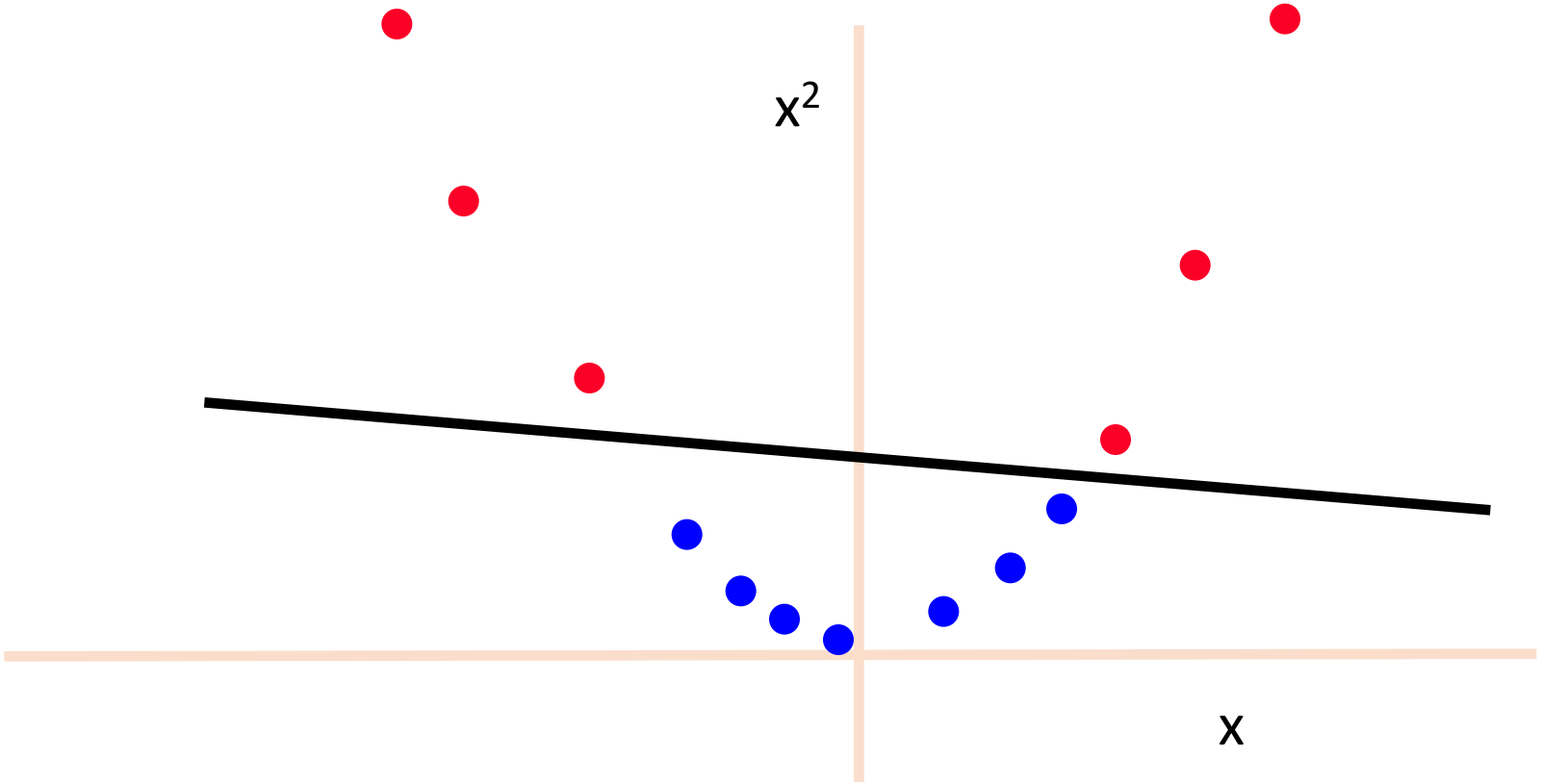
- Data are not linearly separable in one dimension
- Not separable if you insist on using a specific class of functions



Can we do some mapping to make it linear spreadable?

Blown Up Feature Space

- Data are separable in <x, x^2> space



Blown Up Feature Space

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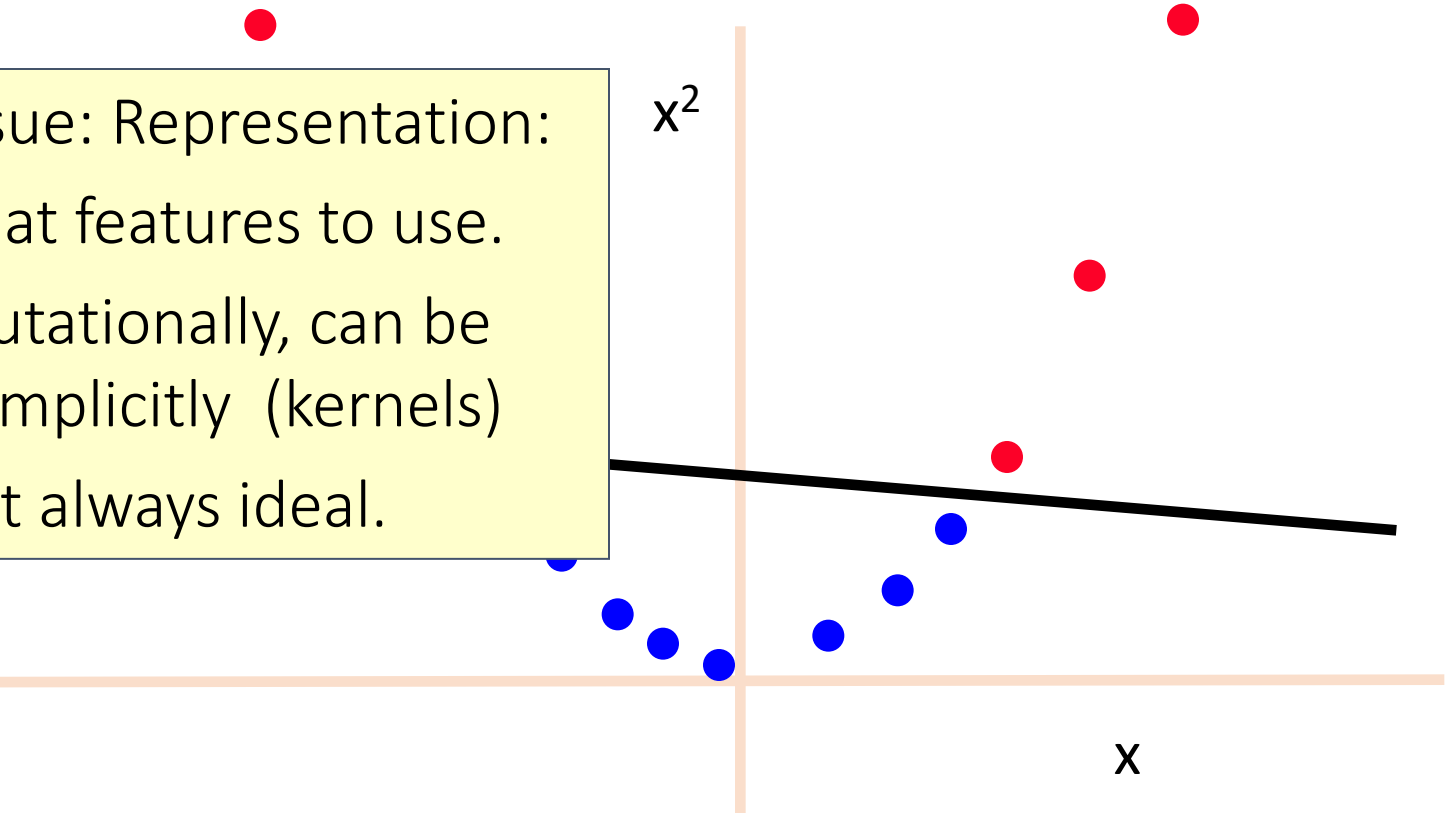


- Key issue: Representation:
  - what features to use.
- Computationally, can be done implicitly (kernels)
  - Not always ideal.

How to learn?

How can we find a good model from the hypothesis space?

Recap: rule-out

1	0	0	1	0	0
2	0	1	0	0	0
3	0	0	1	1	1
4	1	0	0	1	1
5	0	1	1	0	0
6	1	1	0	0	0
7	0	1	0	1	0

m-of-n rules: There are 32 possible rules of the form "y = 1 if and only if at least m of the following n variables are 1"

Notation: 2 variables from the set on the left. **Value**: Index of the counterexample.

variables	1-of	2-of	3-of	4-of
{X1}				
{X2}				
{X3}				
{X4}				
{X1,X2}				
{X1, X3}				
{X1, X4}				
{X2,X3}	2	3	-	-

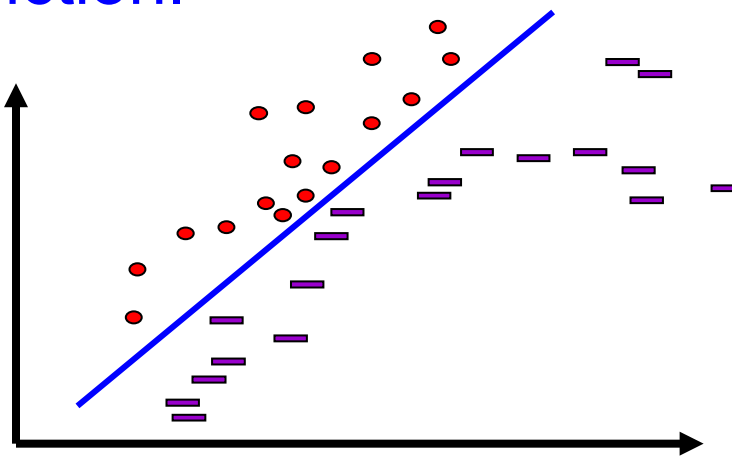
variables	1-of	2-of	3-of	4-of
{X1,X2,X3,X4}				3

Learning is the removal of our remaining uncertainty

Found a consistent hypothesis.

How about linear function?

- Challenges
  - The hypothesis space contains infinite # functions
  - Several functions are consistent with the data
- A possibility: Local search
  - Start with a linear threshold function.
  - See how well you are doing.
  - Correct
  - Repeat until you converge.



Search can be done in a smarter way

- There are other ways that do not search directly in the hypotheses space
- Directly compute the hypothesis by optimizing an objective

- Key question: what is a good classifier?

General Framework for Learning

Problem Setting

- Set of possible instances X
- Set of possible labels Y
- Unknown target function f : X ➔ Y
- Set of function hypotheses $H = \{h \mid h : X \rightarrow Y\}$

Input: Training instances drawn from data generating distribution p

$$\{(x_i, y_i)\}_{i=1}^{n} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$$

Output: Hypothesis h in H that best approximates f

Learning Problem

Output: Hypothesis *h* in *H* that best approximates *f*

h should do well (as measured by the loss) on future instances

Formally, *h* should have low expected (test) loss/Risk

$$\mathbb{E}_{(x,y)\sim p}\left[L(y,h(x))\right] = \sum_{x,y} p(x,y)L(y,h(x))$$

Problem?

We don't know what *p* is

But we are given samples drawn from *p*

Slide credit: Eric Eaton
Based on slide by Tom Mitchell

Learning Problem

We instead approximate the risk by the training error/ empirical risk

$$\frac{1}{n}\sum_{i=1}^{n} L(y_i, h(x_i))$$

When is this reasonable ?

Both the training data **and** the test set are generated based on this distribution

$D = \{x_i, y_i\}_{i=1}^{n}$ is called training data

Challenges

1. Minimizing. $\frac{1}{n}\sum_{i=1}^{n} L(y_i, h(x_i))$ is in general a NP-hard problem

2. Can make the training error zero by memorizing if the hypothesis space is expressive.

Challenges

1. Minimizing. $\frac{1}{n}\sum_{i=1}^{n} L(y_i, h(x_i))$ is in general a NP-hard problem
   - Think of the
   - To alleviate this computational problem, minimize a new function – a convex upper bound of the classification error function

1. Can make the training error zero by memorizing if the hypothesis space is expressive.

Algorithmic View of Learning: an Optimization Problem

- A **Loss Function** L(h(x),y) measures the penalty incurred by a classifier h on example (x,y).
- There are many different loss functions one could define:
  - Misclassification Error:

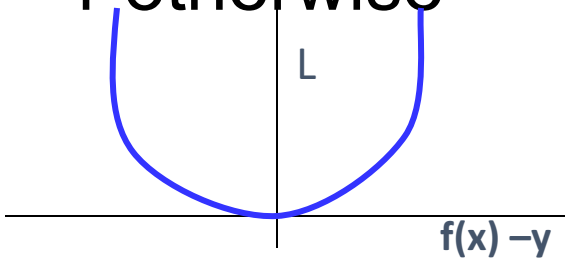
    $L(h(x),y) = 0$ if $h(x) = y$; 1 otherwise

  - Squared Loss:

    $L(h(x),y) = (h(x) - y)^2$

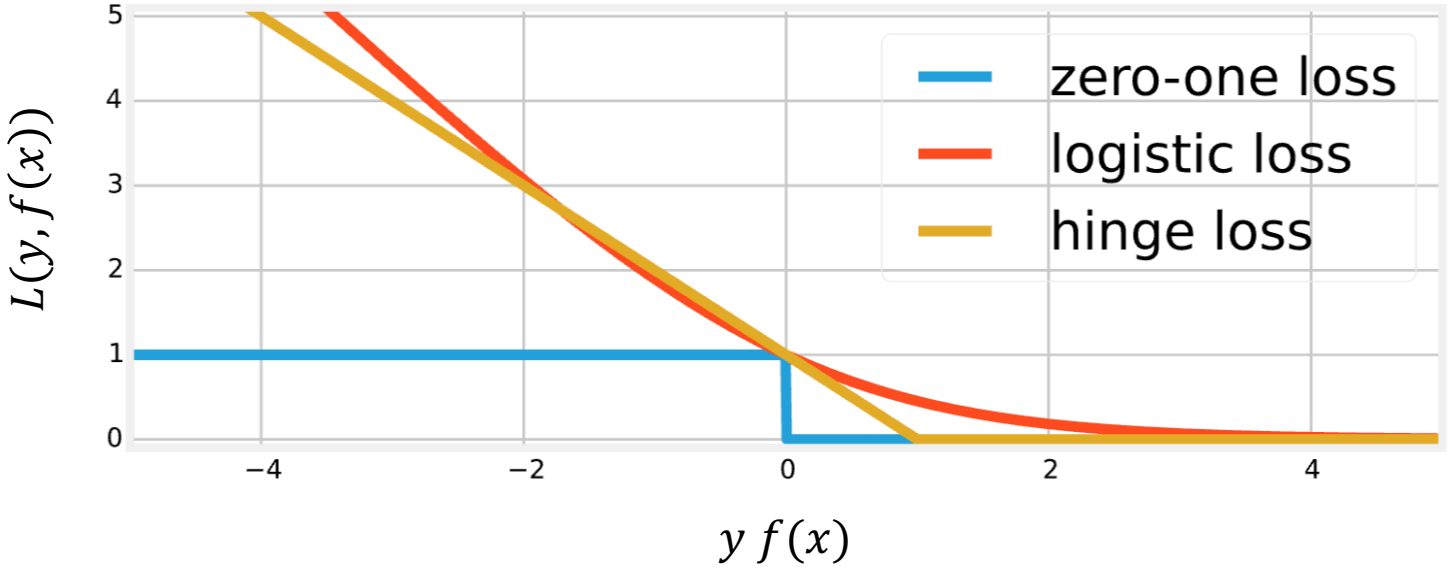
  - Input dependent loss:

    $L(h(x),y) = 0$ if $f(x) = y$; $c(x)$ otherwise.



How about the loss function?

- Usually, we cannot minimize 0-1 loss
  - It is a combinatorial optimization problem: NP-hard
- Idea: minimizing its upper-bound



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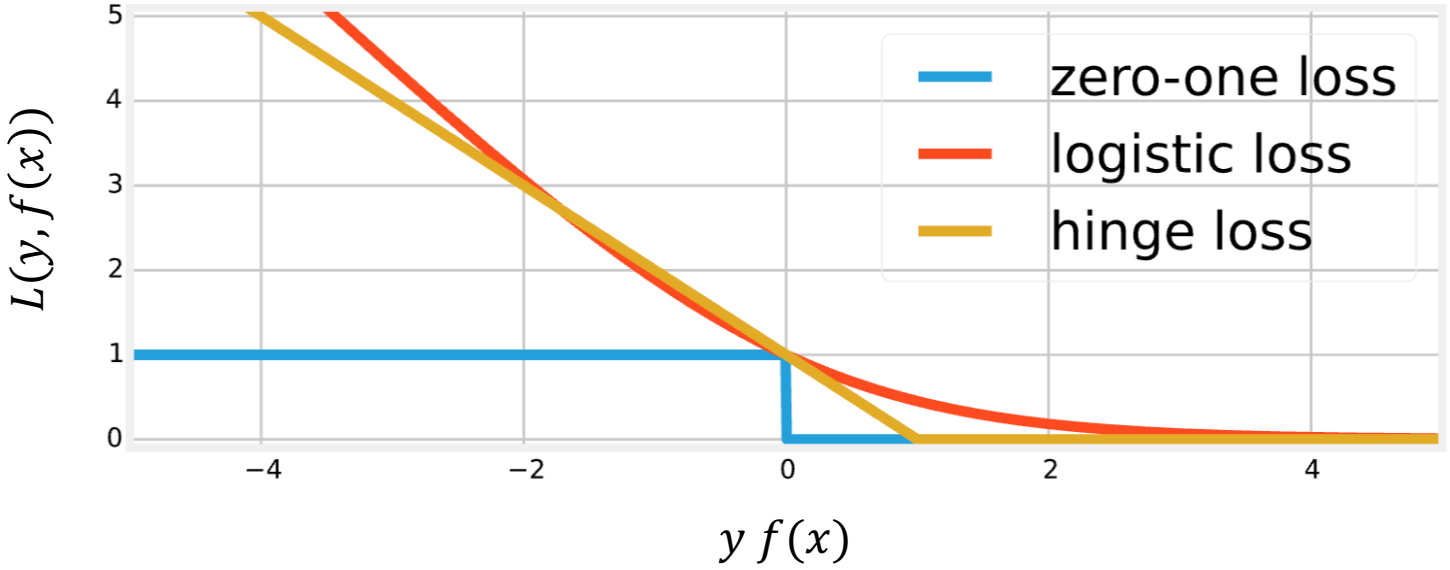
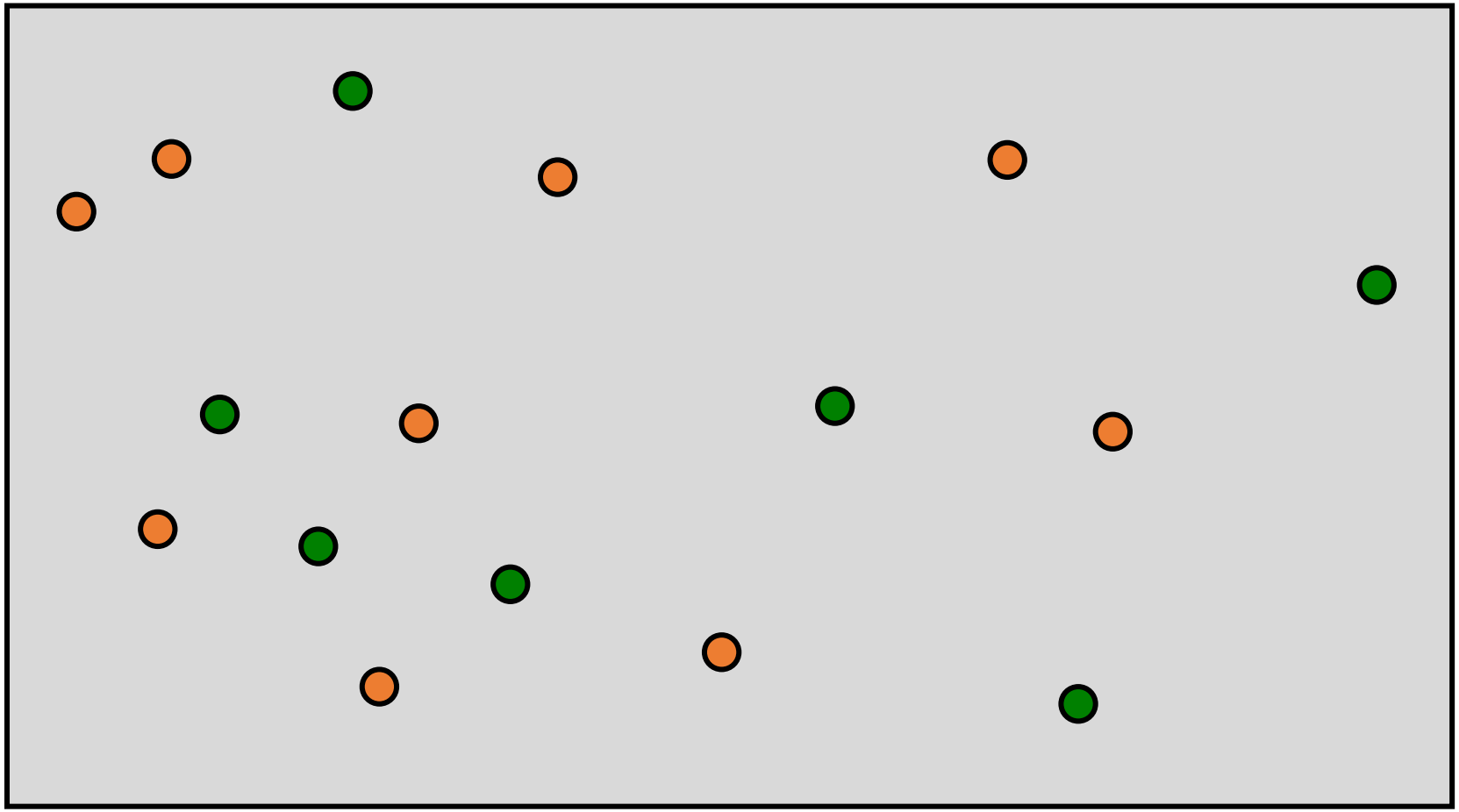


Challenges

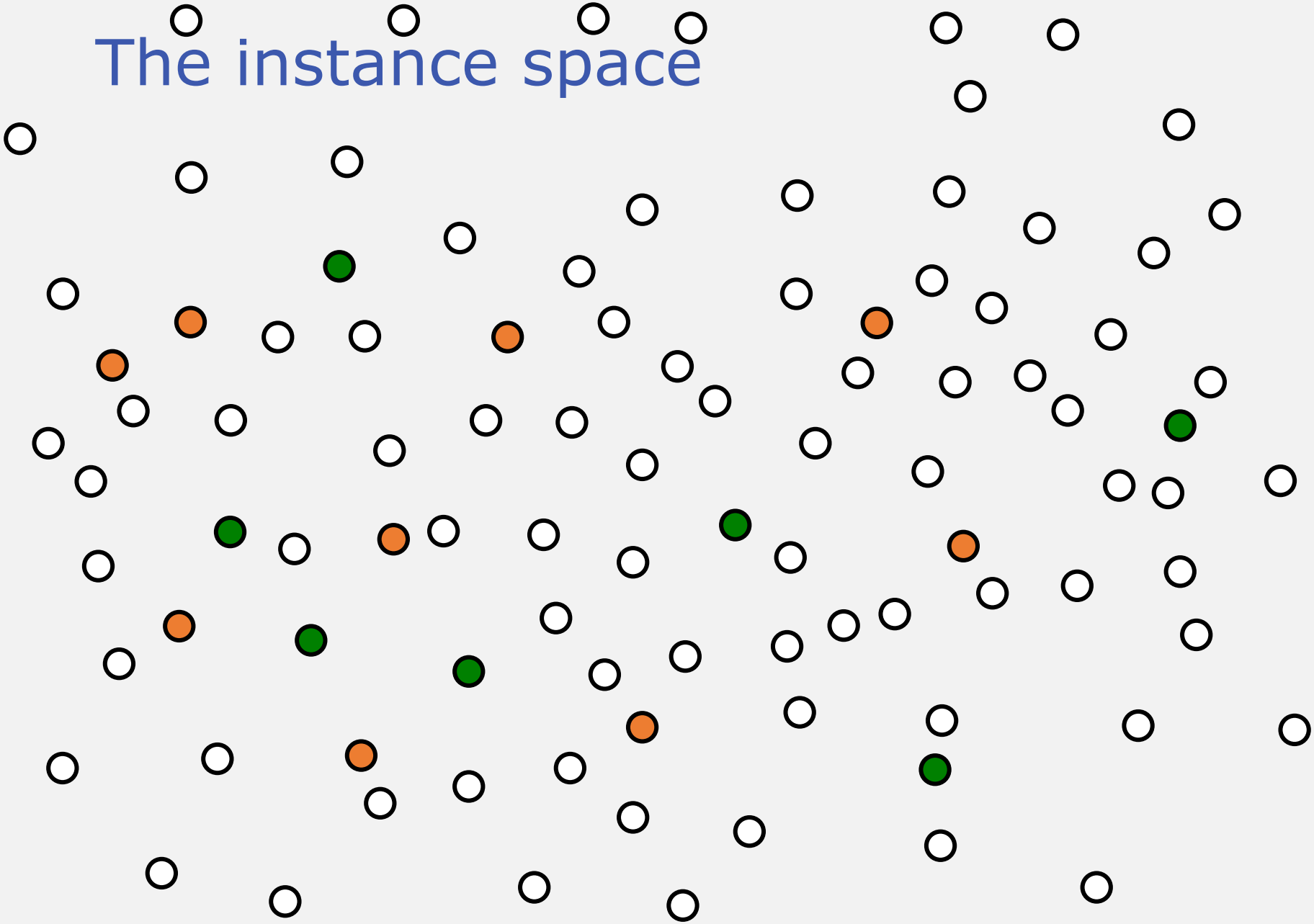
1. Minimizing. $\frac{1}{n}\sum_{i=1}^{n} L(y_i, h(x_i))$ is in general a NP-hard problem
   - **To alleviate this computational problem, minimize a new function – a convex upper bound of the classification error function**

2. Can make the training error zero by memorizing if the hypothesis space is expressive.

Our training data

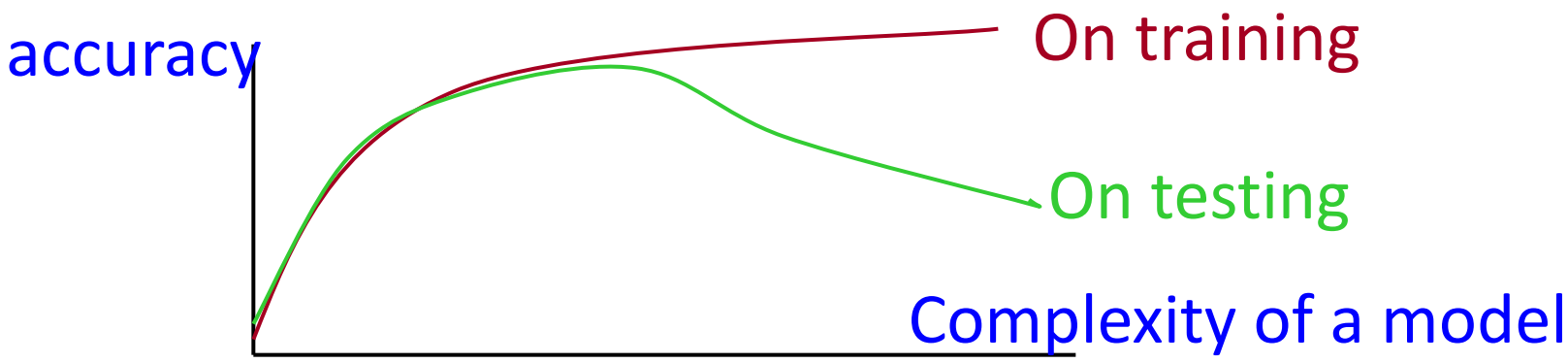


The instance space



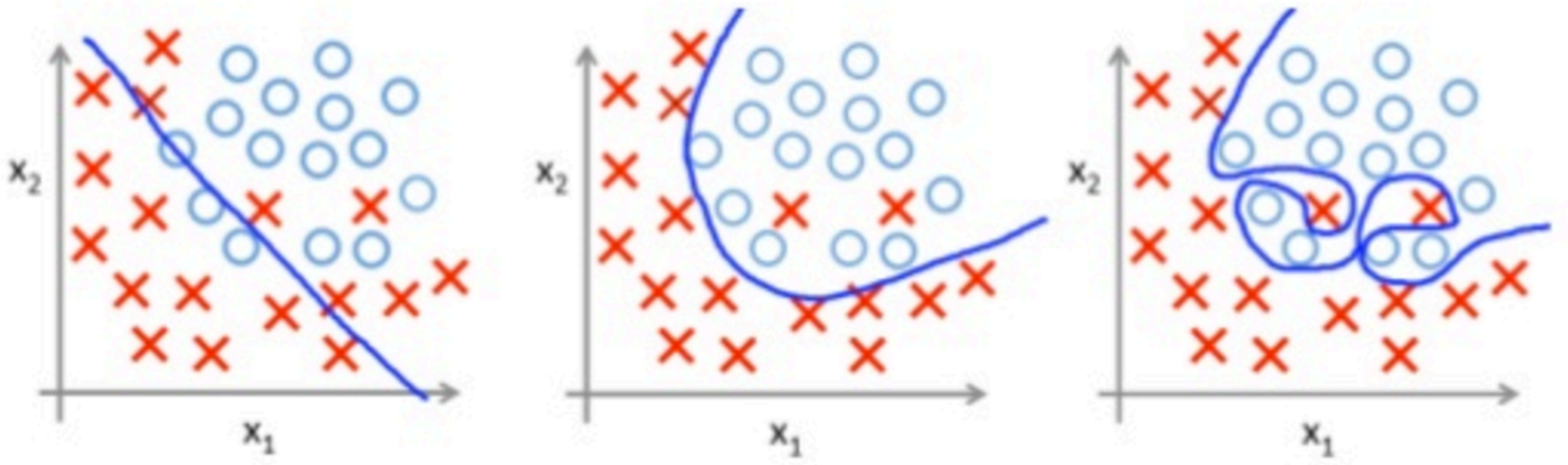
Overfitting the Data

- Learning a tree that classifies the training data perfectly may not lead to the tree with the best generalization performance.
  - There may be noise in the training data
  - The algorithm might be making decisions based on very little data



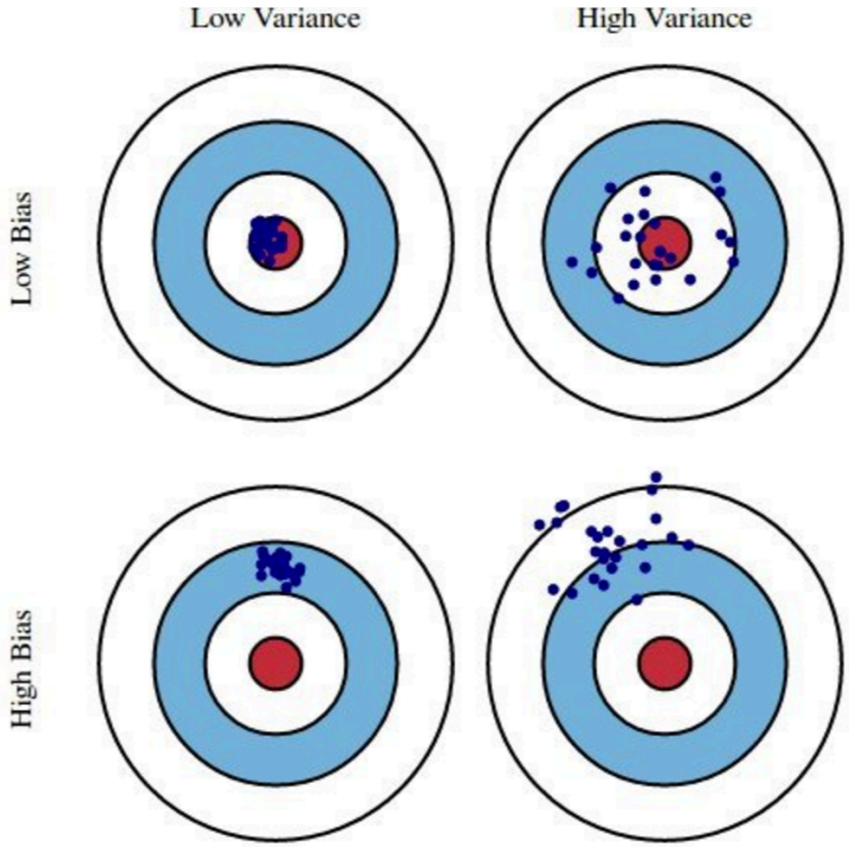
Under-fitting and over-fitting

- Which classifier (blue line) is the best one?



Bias V.S. Variance

- Remember, training data are subsamples drawn from the true distribution
- Exam strategy:
  - Study every chapter well
    - A+: Low var & bias
  - Study only a few chapters
    - A+? B? C? Low bias; High var
  - Study every chapter roughly
    - B+: Low var; high bias
  - Go to sleep
    - B ~D: High var, high bias



Prevent overfitting

- Using a less-expressive model
  - E.g., linear model
- Adding regularization
  - Promote simper models
- Data perturbation
  - Make the model more robust
  - Can be done algorithmically (e.g., dropout)
- Stop the optimization process earlier
  - Sounds bad in theory; but works in practice.

Machine Learning Practice

Putting it all together:

Develop ML algorithms

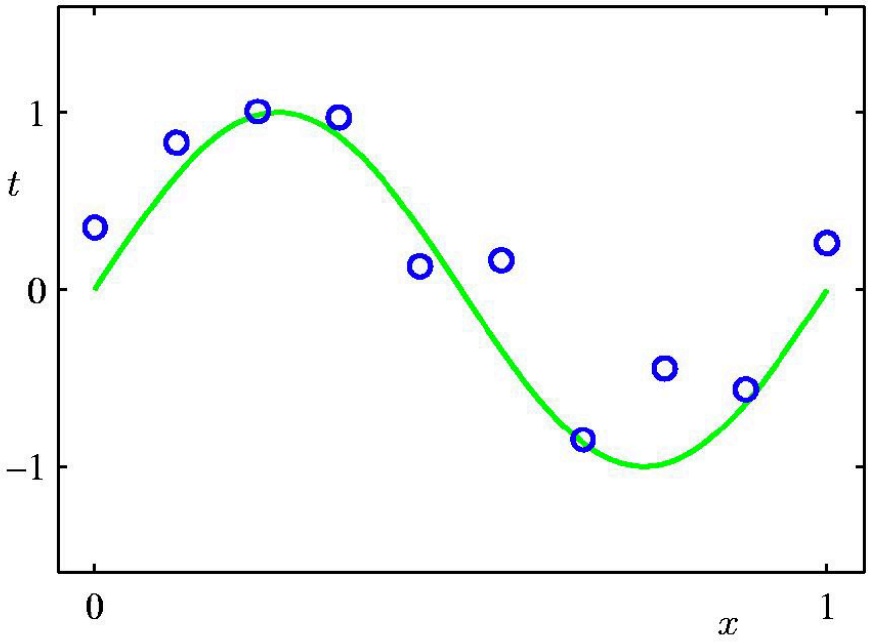
- Step 1: Collect data
- Step 2: Design your algorithm
- Step 3: Verify your algorithm; tune hyper-parameters
  - Option 1: Split data to Train/Dev
  - Option 2: use Cross-Validation
- Step 4: Retrain the model using the best parameter on the whole dataset
- Step 5: Deploy your model on real test data

Example: Regression Problem

- Consider simple regression dataset
  - $f : X \rightarrow Y$
  - $x \in R$
  - $y \in R$

- Question 1: How should we pick the hypothesis space H ?
- Question 2: How do we find the best h in this space?

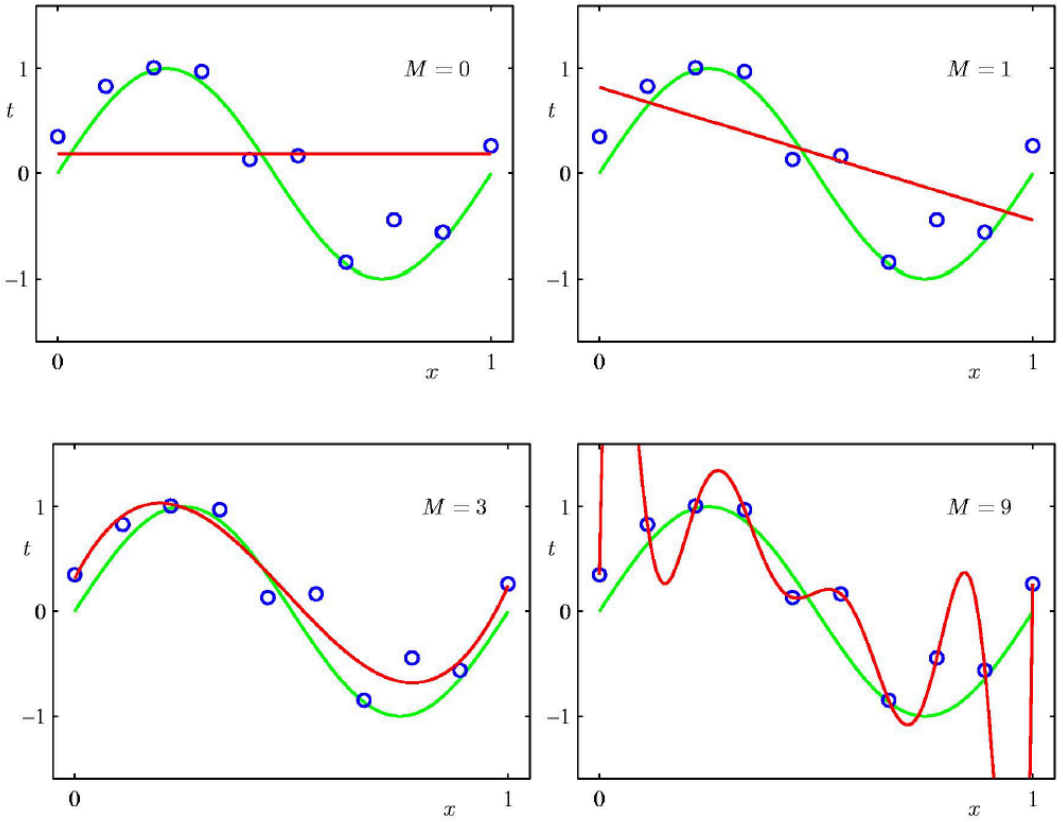
Dataset: 10 points generated from sin function with noise



Based on slide by David Sontag
Images from Bishop [PRML]

Hypothesis Space: Degree-M Polynomials

- Infinitely many hypotheses
- Which one is **best**?



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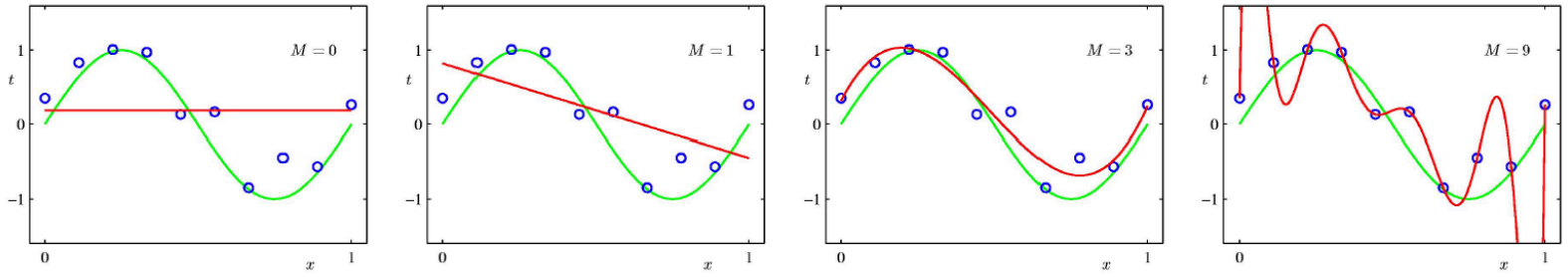
Hypothesis Space: Degree-M Polynomials

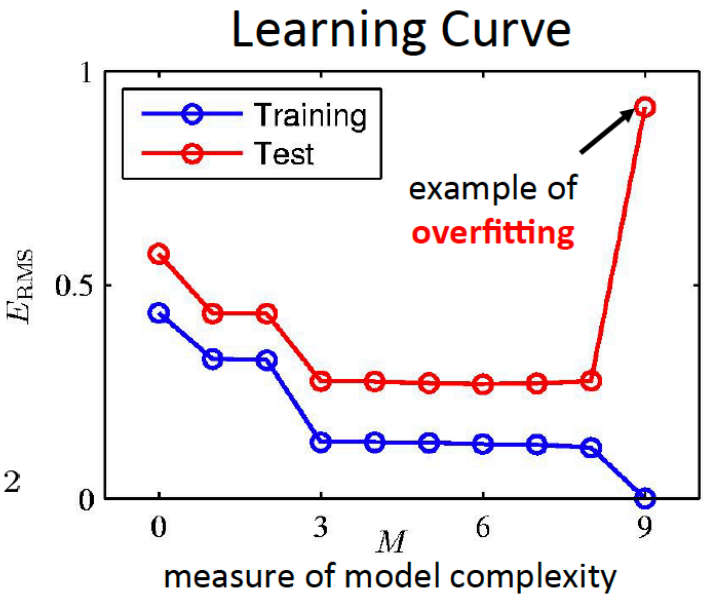


- For regression, common choice is squared loss

$$L(y_i, h(x_i)) = (y_i - h(x_i))^2$$

- *Empirical loss* of function *h* applied to training data is then

$$\frac{1}{n}\sum_{i=1}^{n} L(y_i, h(x_i)) = \frac{1}{n}\sum_{i=1}^{n} (y_i - h(x_i))^2$$



Based on slide by David Sontag
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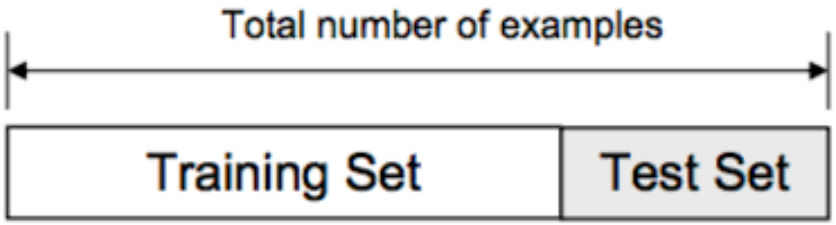
How to find the best M?

- There are two types of parameters
  - Hyper-parameters (e.g., M) need to be tuned
  - Model parameters that can be learned from the training set
- M is a hyper-parameter for the regression model
- We can try out different M and see which one work
- How to?

Train/Dev splits



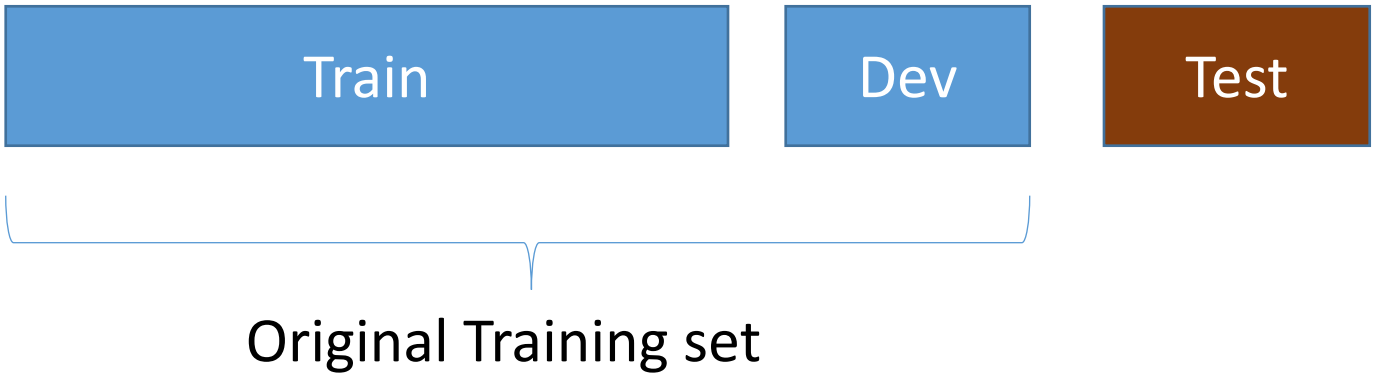
- Usually a data set consists of a training set (for learning) and a test set (for evaluation)

- You need to report performance on test data, but you are not allowed to look at it.
  - Why?
  - You are allowed to look at the development data (and use it to tweak parameters)

Train/Dev splits

Dev is like mock exam

- Further split your training data into two sets:
  - Training data (often 70-90%)
  - Development data (10-20%)



Trade off in Train/Dev splits

- Large Train, small Dev
  (e.g., #train = 48, #dev = 2)

Result on dev is not representative

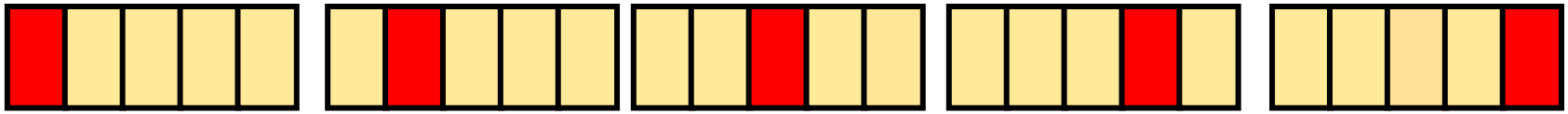
- Small Train, Large Dev
  (e.g., #train = 30, #dev = 20)

May not have enough data to train a model

N-fold cross validation (useful esp. when training set is small)

- Instead of a single test-training split:

- Split data into N equal-sized parts

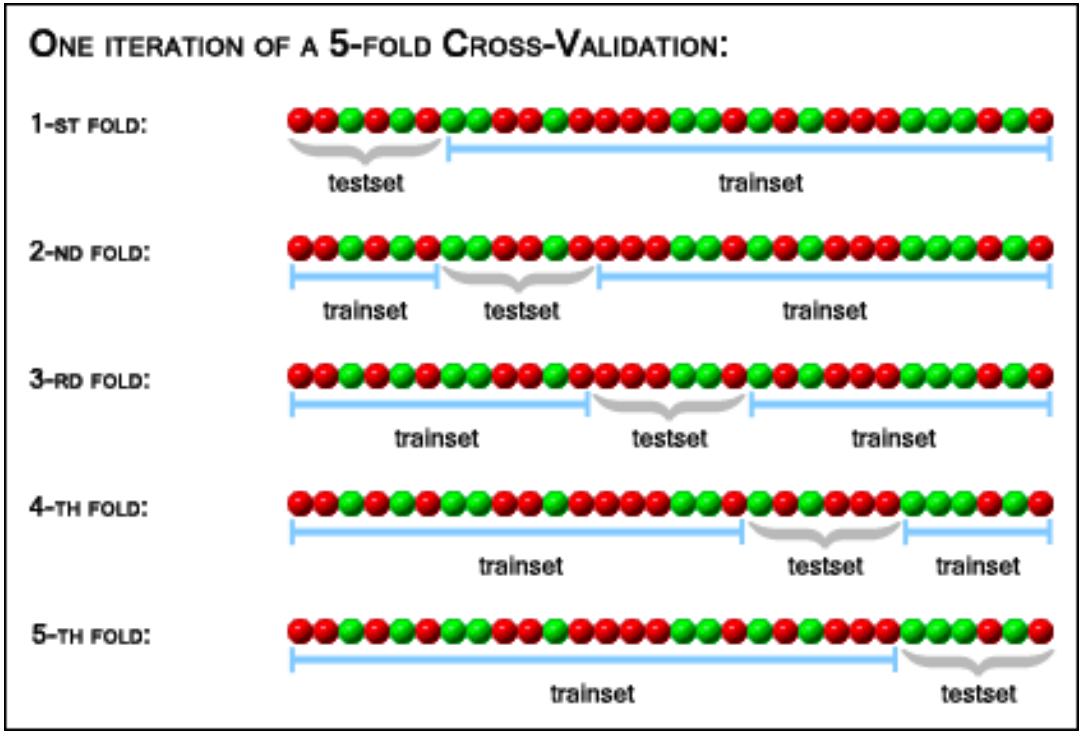


- Train and test N different classifiers
- Report average accuracy and standard deviation of the accuracy to choose parameters

Finding parameters based on cross validation

- Given D^{TRAIN} and D^{TEST}, for each possible value of the hyper-parameter (e.g., M = 1,2, 3,…,10)
  - Conduct cross validation on D^{TRAIN} with parameter K
- Choose the model parameter with the best cross validation performance
- Re-train the model on D^{TRAIN} with the best parameter set
- Evaluate the model on D^{TEST}

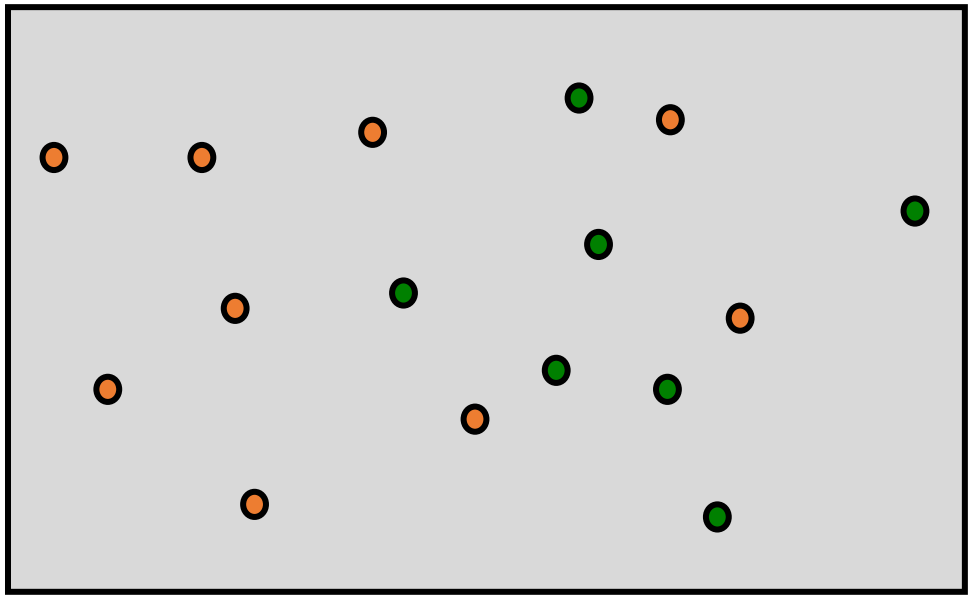
Example



	Parameter 1	Parameter 2
	Accuracy: 100%	Accuracy: 100%
	Accuracy: 50%	Accuracy: 100%
	Accuracy: 50%	Accuracy: 100%
	Accuracy: 100%	Accuracy: 100%
	Accuracy: 100%	Accuracy: 50%
	Avg Accuracy: 80%	Avg Accuracy: 90%

In class-practice

- Consider two class classifiers:
  - Vertical line; Horizontal line
  - Which one is better on the following dataset?



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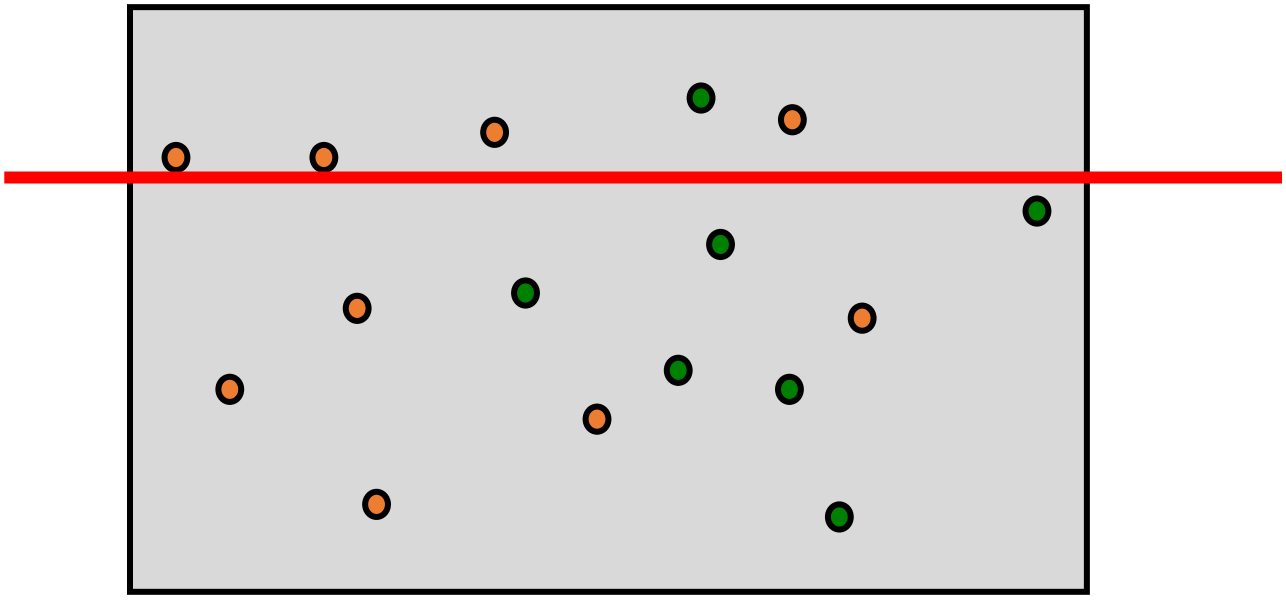
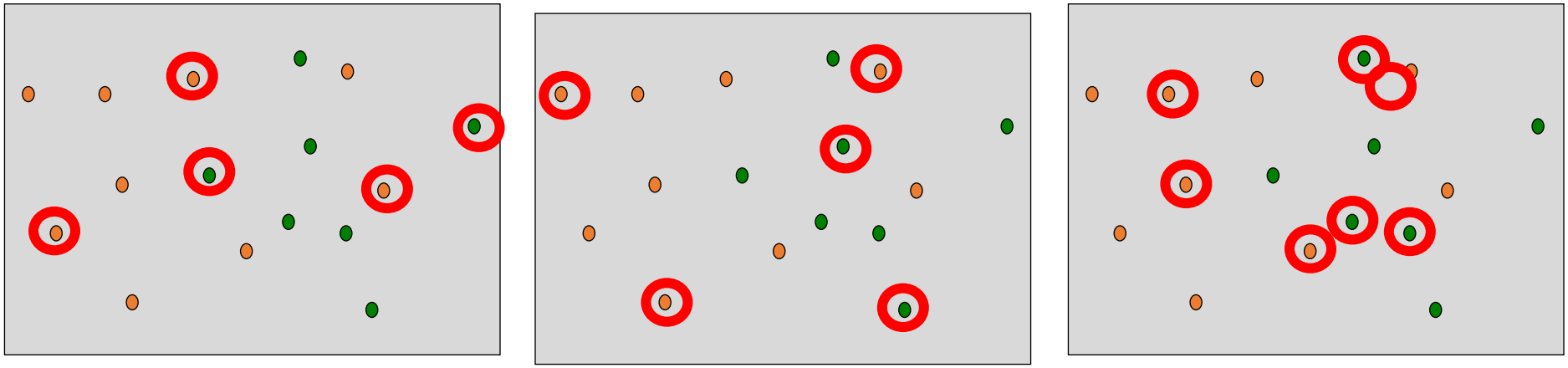


In class-practice

- Consider two class classifiers:
  - Vertical line; Horizontal line
  - Which one is better on the following dataset?
  - Three-fold cross validation



Machine learning libraries

- Machine learning toolbox:
  - Scikit learn (python), Weka (java), many others.
- Deep learning models
  - Pytorch, DyNet, Tensorflow
- Big data
  - Apache spark
- Many others …

Playground & Resources

- Tutorial:
  - https://pytorch.org/tutorials/
  - http://scikit-learn.org/stable/tutorial/index.html
- ML competitions:
  - https://www.kaggle.com/ (several others)
- Conferences/Papers:
  - ICML / NIPS / AAAI/ IJCAI/ ICLR/ …

Practical tricks

- Make sure you can reproduce your experiments
  - Set random seed; Keep exp log; Use code repository (e.g., Github)
  - Use configure file to manager parameters
  - Script for finding parameters
- Start with small data
  - Split a tiny dataset for debugging
  - Split a small dataset to check which parameters are important; Some hyper-parameters do not depend on size of data (in theory)