Supervised Learning (COMP0078)

1. Introduction to supervised learning

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(Slides thanks to Mark Herbster)

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References

Useful References

- *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*, T. Hastie, R. Tibshirani, & J. Friedman, Springer (2009)
- *Understanding Machine Learning from Theory to Algorithms*, S. Shalev-Shwartz and S. Ben-David, Cambridge University Press (2014)
- *Convex Optimization*, S. Boyd and L. Vandenberghe (2004)
- *Kernel Methods for Pattern Analysis*, J. Shawe-Taylor, and N. Cristianini, Cambridge University Press (2004)
- *Pattern Recognition and Machine Learning*, C. Bishop, Springer (2006)

Course information

1. When
   - Thursdays 1:30-2:30 pm [Office Hours (Teams)]
   - Thursday 4-5 pm [Q+A with TA]
     OPTIONAL (But recommended!)]

2. Questions :
   - Moodle forum
   - `sl-support@cs.ucl.ac.uk`

3. TAs:
   - Antonin Schrab
   - Ming Liang Ang

Assessment

1. Coursework (50%) and Exam (50%)
2. 2 courseworks assignments
   (deliver them on-time, penalty otherwise)
3. To pass the course, you must obtain an average of at least 50% when the homework and exam components are weighted together (MSc ML/CSML/DSML). MENG and other degrees check with your programme coordinator.

Prerequisites

- Calculus (real-valued functions, limits, derivatives, Taylor series, integrals,...)
- Elements of probability theory (random variables, expectation, variance, conditional probabilities, Bayes rule,...)
- Fundamentals of linear algebra (vectors, angles, matrices, eigenvectors/eigenvalues,...),
- A bit of optimization theory (convex functions, Lagrange multipliers)

Antonin (one the TAs), will give a Math “boothcamp” on the first TA session (Next Thursday, Oct 12).

Provisional course outline

- (Lecture 1) Key concepts (probabilistic formulation of learning from examples, loss function, learning algorithm, overfitting and underfitting, model selection, cross validation); two basic learning algorithms linear regression and $k-$NN;
- (Lecture 2) Regularisation, Kernels
- (Lecture 3) Support Vector Machines
- (Lecture 4) Decision Trees and Ensemble Learning
- (Lecture 5) Online Learning I

Provisional course outline

- (Lecture 6) Graphs in Machine Learning
- (Lecture 7) Learning Theory
- (Lecture 8) Online Learning II
- (Lecture 9) Matrix Completion (time permitting)

This week's plan

- The supervised learning problem
- Two learning algorithms: least squares and k-NN
- Probabilistic model, error function, optimal solutions
- Bias-Variance tradeoff, NFL theorems
- Asymptotic Optimality of k-NN
- Hypothesis space, overfitting and underfitting
- Choice of the learning algorithm (Model selection)

Supervised Learning Problem

Given a set of **input/output** pairs (**training set**) we wish to compute the functional relationship between the input and the output

$$\boldsymbol{x} \longrightarrow \boxed{f} \longrightarrow y$$

- **Example 1:** (people detection) given an image we wish to say if it depicts a person or not. The output is one of 2 possible categories
- **Example 2:** (pose estimation) we wish to predict the pose of a face image The output is a continuous number (here a real number describing the face rotation angle)

In both problems the input is a high dimensional vector $\boldsymbol{x}$ representing pixel intensity/color

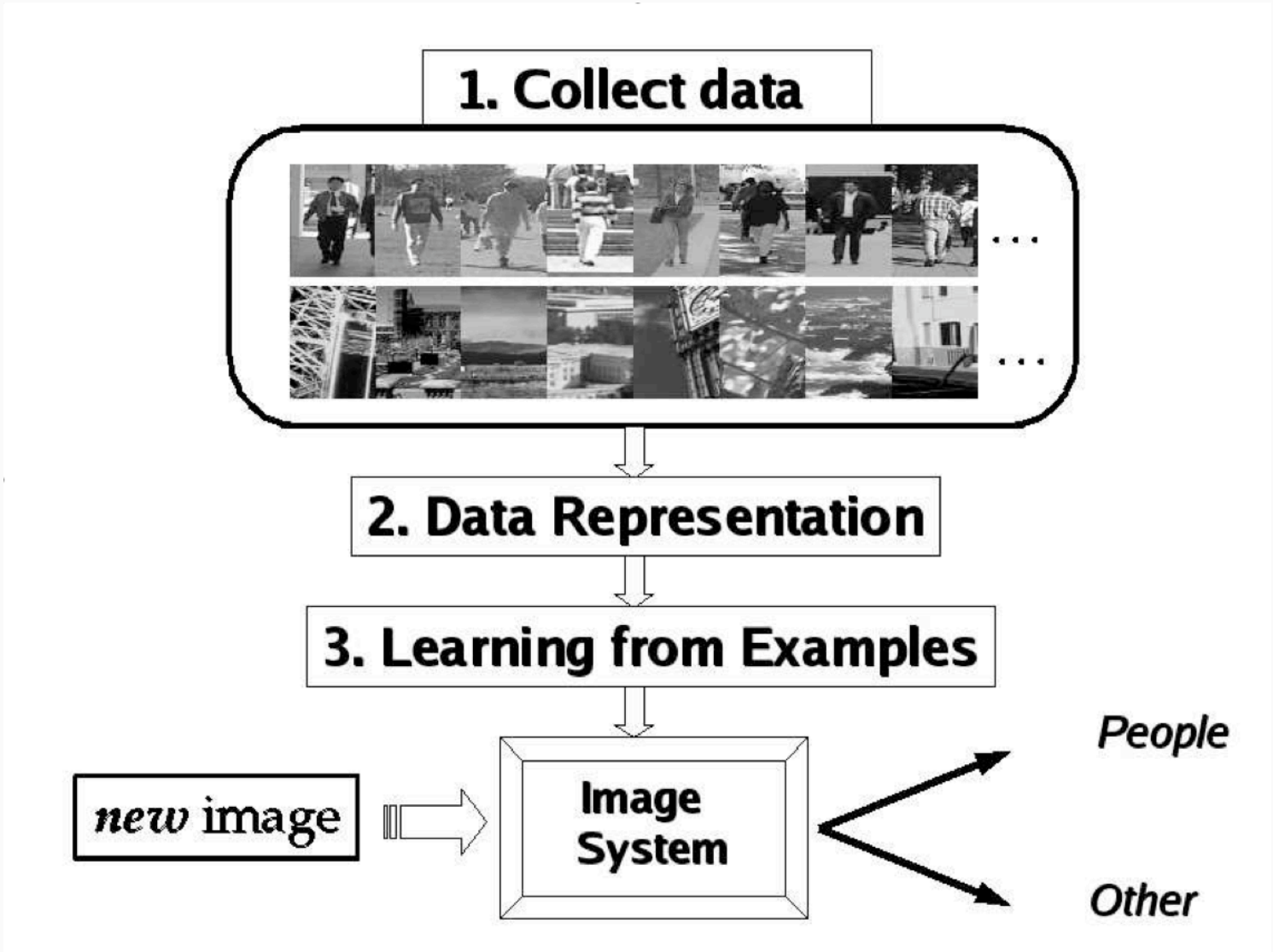
Why and when learning?

- The aim of learning is to develop software systems able to perform particular tasks such as people detection.
- Standard software engineering approach would be to specify the problem, develop an algorithm to compute the solution, and then implement efficiently.
- Problem with this approach is developing the algorithm:
  - No known criterion for distinguishing the images;
  - In many cases humans have no difficulty;
  - Typically problem is to specify the problem in logical terms.

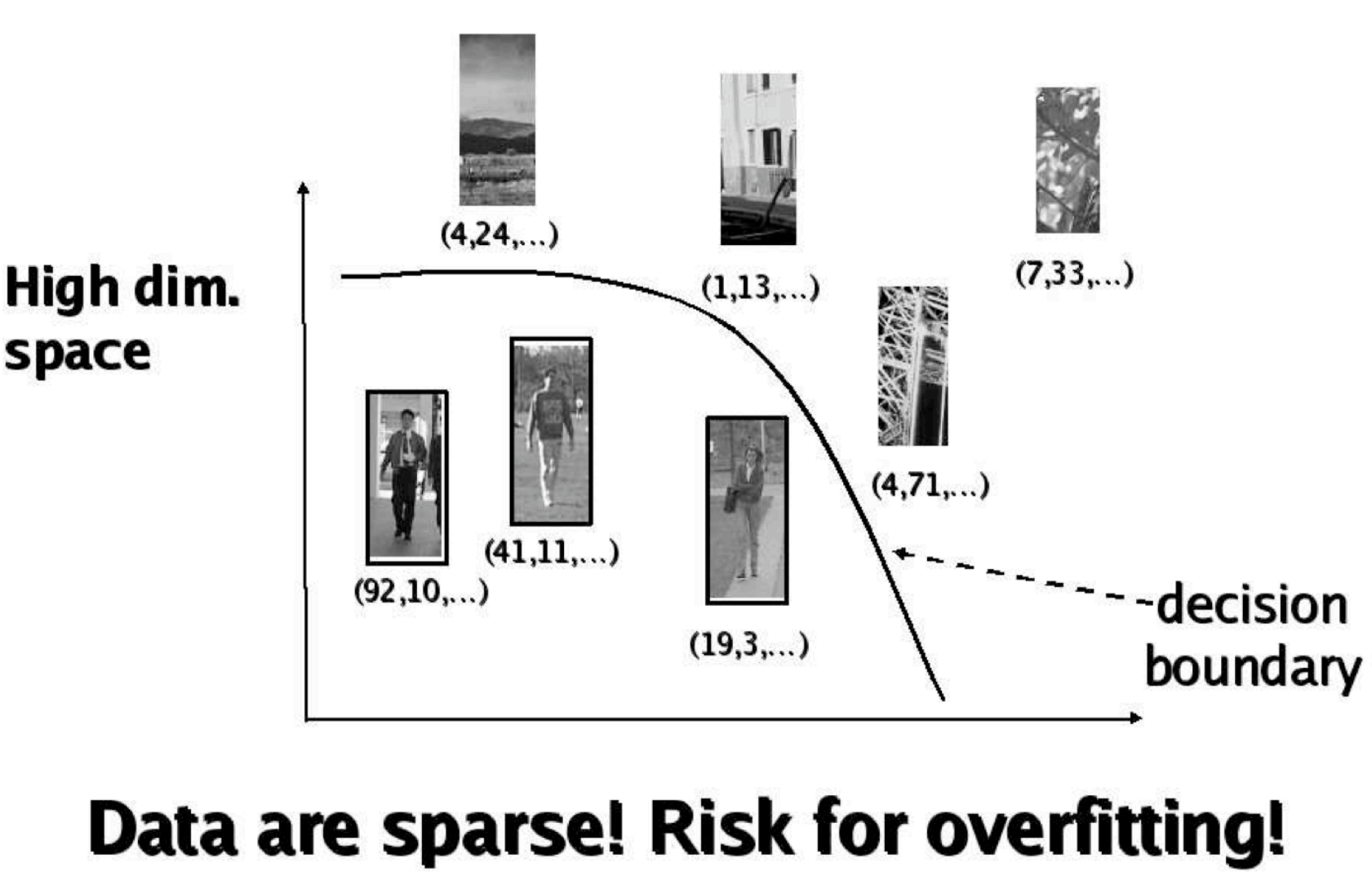
Learning approach

- Learning attempts to infer the algorithm for a set of (labelled) examples in much the same way that children learn by being shown a set of examples (eg sports/non sports car).
- Attempts to isolate underlying structure from a set of examples. Approach should be
  - stable: finds something that is not chance part of set of examples
  - efficient: infers solution in time polynomial in the size of the data
  - robust: should not be too sensitive to mislabelled/noisy examples

People Detection Example



People detection example (cont.)



Supervised Learning Model

- Goal: Given training data (pattern,target) pairs

$$S = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$$

infer a function f_S such that

$$f_S(\boldsymbol{x}_i) \approx y_i$$

for the future data

$$S' = \{(\boldsymbol{x}_{m+1}, y_{m+1}), (\boldsymbol{x}_{m+2}, y_{m+2}), \ldots\}.$$

- Classification : $y \in \{-1, +1\}$; Regression : $y \in \mathbb{R}$
- $\mathcal{X}$: input space (eg, $\mathcal{X} \subseteq \mathbb{R}^n$), with elements $\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{x}_i, \ldots$
- $\mathcal{Y}$: output space, with elements $y, y', y_i, \ldots$

Supervised learning problem: compute a function which “best describes” I/O relationship

Learning algorithm

- Training set: $S = \{(\boldsymbol{x}_i, y_i)_{i=1}^m\} \subseteq \mathcal{X} \times \mathcal{Y}$
- A **learning algorithm** is a mapping $S \mapsto f_S$
- A new input $\boldsymbol{x}$ is predicted as $f_S(\boldsymbol{x})$

Example Algorithms

- Linear Regression
- Neural Networks
- Decision Trees
- Support Vector Machines

- In the course we mainly deal with deterministic algorithms but we'll also comment on some randomized ones
- Today: we describe two simple learning algorithms: *linear regression and k−nearest neighbours*

Some Questions

- How is the data **collected**? (need assumptions!)
- How do we **represent** the inputs? (may require preprocessing step)
- How **accurate** is f_S on new data (study of **generalization error**)?
- Many algorithms may exist for a task. How do we choose?
- How "**complex**" is a learning task? (computational complexity, sample complexity)

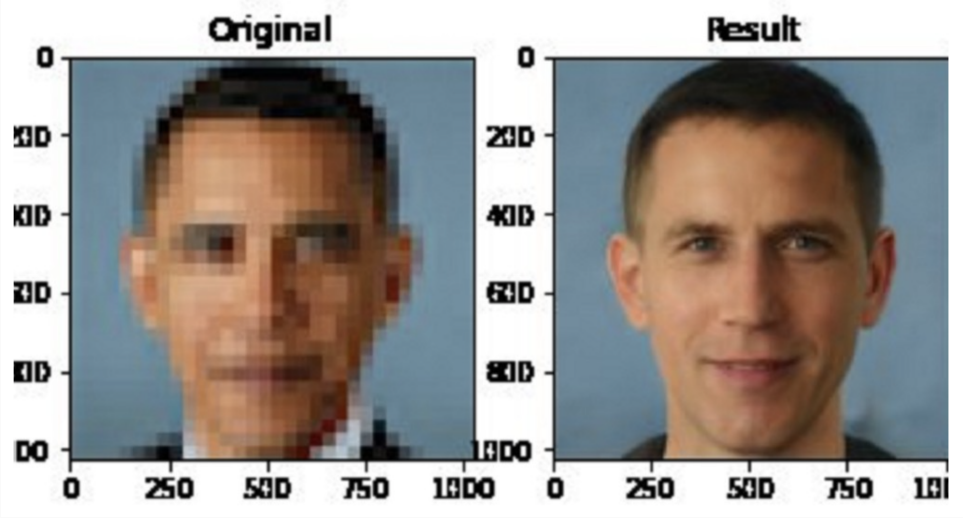
Data Ethics [Not Examined]

The New York Times

There Is a Racial Divide in Speech-Recognition Systems, Researchers Say

Technology from Amazon, Apple, Google, IBM and Microsoft misidentified 35 percent of words from people who were black. White people fared much better.

Amazon's Echo device is one of many similar gadgets on the market. Researchers say there is a racial divide in the usefulness of speech recognition systems. Grant Hindsley for The New York Times



For an introductory discussion see this talk by Emily Denton &Timnit Gebru

Slides: `https://drive.google.com/file/d/1IvUgCTUciIJQ-dIqQAYNO11X3guzqnYN/view`

Talk: `https://youtu.be/v_XBJd1Fxqc`

Some difficulties/aspects of the learning process

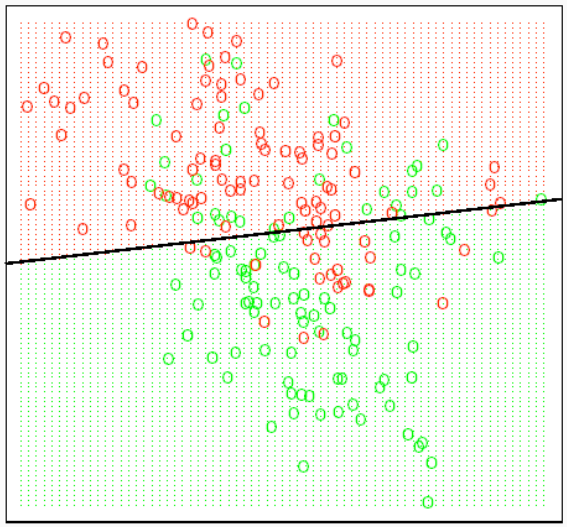
- New inputs **differ** from the ones in the training set (look up tables do not work!)
- Inputs are measured with **noise**
- Output is **not deterministically** obtained by the input
- Input is often **high dimensional** but some components/variables may be irrelevant
- How can we incorporate **prior knowledge**?

Binary classification: an example

We describe two basic learning algorithms/models for classification which can be easily adapted to regression as well. We choose: $\mathcal{X} = \mathbb{R}^2$, $\boldsymbol{x} = (x_1, x_2)$ and $\mathcal{Y} = \{\textit{green}, \textit{red}\}$

Our first learning algorithm computes a **linear function**, $\boldsymbol{w}^\top \boldsymbol{x} + b$ and classifies an input $\boldsymbol{x}$ as

$$f(\boldsymbol{x}) = \begin{cases} \texttt{red} & \boldsymbol{w}^\top \boldsymbol{x} + b > 0 \\ \texttt{green} & \boldsymbol{w}^\top \boldsymbol{x} + b \leq 0 \end{cases}$$



Linear Regression (Least Squares)

- Emerged in response to problems in Astronomy and Navigation
- Motivated by the need to combine multiple noisy measurements
- Method first described by Gauss in 1794

A Simple Problem – 1

Given the data set

$$S = \{((1, 1), 3), ((2, 3), 7)\}$$

Then with the new input $\boldsymbol{x}_3 = (4, 2)$

how should we predict y_3?

Why? What Assumptions?

A Simple Problem – 2

Model as a system of equations

$$\begin{aligned} w_1 + w_2 &= 3 \\ 2w_1 + 3w_2 &= 7 \end{aligned}$$

or more directly as

$$X\boldsymbol{w} = \mathbf{y}$$

with

$$X = \begin{pmatrix} 1 & 1 \\ 2 & 3 \end{pmatrix}; \qquad \mathbf{y} = \begin{pmatrix} 3 \\ 7 \end{pmatrix}$$

A Simple Problem – 3

Solving in matlab

$$\boldsymbol{w} = X^{-1}\mathbf{y}$$

```
>> y = [3 ; 7]
y = 3
    7
>> X = [1,1 ; 2, 3]
X = 1     1
    2     3
>> XI = X^(-1)
XI = 3    -1
    -2     1
>> w= XI * y
w = 2
    1
>> w= X \ y %% More efficient than calculating inverse use in practice see help mldivide
w = 2
    1
```

We now have the linear predictor

$$\hat{y} = \boldsymbol{w} \cdot \boldsymbol{x}$$

Thus predict $\hat{y}_3 = \boldsymbol{w} \cdot \boldsymbol{x}_3 = w_1 x_{3,1} + w_2 x_{3,2} = 4 \times 2 + 1 \times 2 = 10.$

A Simple Problem – 4

What if?

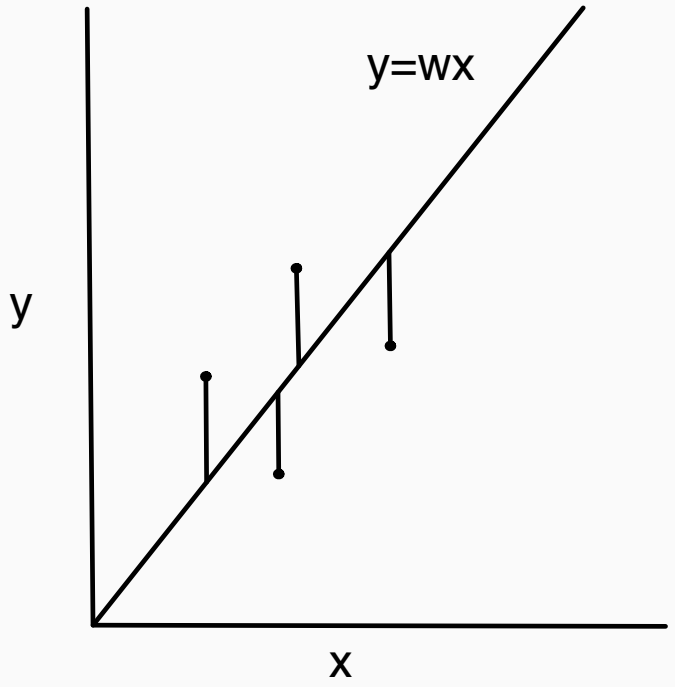
- Overdetermined:

$$S = \{((1,1),3),((2,3),7),((2,1),3)\}$$

- Underdetermined:

$$S = \{((1,1,2),3),((2,4,3),7)\}$$

Minimize square error – 1



Find a linear predictor $\hat{y} = \boldsymbol{w} \cdot \boldsymbol{x}$ to minimize the square error over the data $\mathcal{S} = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$ thus

$$\text{Minimize: } \sum_{i=1}^{m} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{m} (y_i - \boldsymbol{w} \cdot \boldsymbol{x}_i)^2$$

Minimize square error – 2

Thus given,

$$\mathcal{S} = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$$

with $\boldsymbol{x} \in \mathbb{R}^n$ we may represent the pattern and target vectors with the matrices

$$X = \begin{pmatrix} x_{1,1} & x_{1,2} & \ldots & x_{1,n} \\ x_{2,1} & x_{2,2} & \ldots & x_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \ldots & x_{m,n} \end{pmatrix} \text{ and } \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

MSE in Matrix Notation

Thus in matrix notation the *empirical* mean (square) error of the linear predictor $\hat{y} = \boldsymbol{w} \cdot \boldsymbol{x}$ on the data sequence $\mathcal{S}$ is

$$\begin{aligned}
\mathcal{E}_{\text{emp}}(\mathcal{S}, \boldsymbol{w}) &= \frac{1}{m} \sum_{i=1}^{m} (y_i - \hat{y}_i)^2 \\
&= \frac{1}{m} \sum_{i=1}^{m} (y_i - \boldsymbol{w} \cdot \boldsymbol{x}_i)^2 \\
&= \frac{1}{m} \sum_{i=1}^{m} (y_i - \sum_{j=1}^{n} w_j x_{i,j})^2 \\
&= \frac{1}{m} (X\boldsymbol{w} - \mathbf{y})^\top (X\boldsymbol{w} - \mathbf{y})
\end{aligned}$$

MSE minimization. General Case

To compute the minimum we solve for

$$\nabla_{\boldsymbol{w}} \mathcal{E}_{\text{emp}}(\mathcal{S}, \boldsymbol{w}) = \mathbf{0}.$$

recalling that

$$\nabla_{\boldsymbol{w}} = \begin{pmatrix} \frac{\partial}{\partial w_1} \\ \vdots \\ \frac{\partial}{\partial w_n} \end{pmatrix}$$

Thus we need to solve,

$$\nabla_{\boldsymbol{w}} \left[(X\boldsymbol{w} - \mathbf{y})^T (X\boldsymbol{w} - \mathbf{y}) \right] = \mathbf{0}$$

$$\left(\sum_{i=1}^{m} \frac{\partial}{\partial w_1} \left(\sum_{j=1}^{n} X_{ij} w_j - y_i \right)^2, \ldots, \sum_{i=1}^{m} \frac{\partial}{\partial w_n} \left(\sum_{j=1}^{n} X_{ij} w_j - y_i \right)^2 \right)^\top = \mathbf{0}$$

Normal equations

Consider the 2-d case ($n = 2$)

$$\mathcal{E}_{\text{emp}}(\mathcal{S}, \boldsymbol{w}) = \frac{1}{m} \sum_{i=1}^{m} \left(y_i - \boldsymbol{w}^\top \boldsymbol{x}_i\right)^2$$

Note that:

$$\frac{\partial \mathcal{E}_{\text{emp}}(\mathcal{S}, \boldsymbol{w})}{\partial w_k} = \frac{2}{m} \sum_{i=1}^{m} \left(\boldsymbol{w}^\top \boldsymbol{x}_i - y_i\right) \frac{\partial (\boldsymbol{w}^\top \boldsymbol{x}_i)}{\partial w_k} = \frac{2}{m} \sum_{i=1}^{m} \left(\boldsymbol{w}^\top \boldsymbol{x}_i - y_i\right) x_{ik}$$

Hence, to find $\boldsymbol{w} = (w_1, w_2)^\top$ we need to solve the *linear system* of equations

$$\sum_{i=1}^{m} (x_{ik} x_{i1} w_1 + x_{ik} x_{i2} w_2) = \sum_{i=1}^{m} x_{ik} y_i, \quad k = 1, 2$$

Normal equations (cont.)

In vector notations:

$$\sum_{i=1}^{m} \boldsymbol{x}_i \boldsymbol{x}_i^\top \boldsymbol{w} = \sum_{i=1}^{m} \boldsymbol{x}_i y_i$$

In matrix notation:

$$X^\top X \boldsymbol{w} = X^\top \mathbf{y}$$

where

$$X^\top = \begin{bmatrix} x_{11} & \cdots & x_{m1} \\ \vdots & \ddots & \vdots \\ x_{1n} & \cdots & x_{mn} \end{bmatrix} \equiv \left[\boldsymbol{x}_1, \cdots, \boldsymbol{x}_m \right], \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

Least square solution

$$X^\top X \boldsymbol{w} = X^\top \mathbf{y}$$

For the time being we will assume that the matrix $X^\top X$ is invertible, so we conclude that

$$\boldsymbol{w} = (X^\top X)^{-1} X^\top \mathbf{y}$$

Otherwise, the solution may not be unique...

Comment:

In matlab use

$$w = X \backslash y$$

Going back to “b” (adding a bias term)

Substituting $\boldsymbol{x}^\top$ by $(\boldsymbol{x}^\top, 1)$ and $\boldsymbol{w}^\top$ by $(\boldsymbol{w}^\top, b)$, the above system of equations can be expressed in matrix form as (exercise):

$$(\mathbf{X}^\top\mathbf{X})\boldsymbol{w} + \mathbf{X}^\top\mathbf{1}b = \mathbf{X}^\top\mathbf{y}$$
$$\mathbf{1}^\top\mathbf{X}\boldsymbol{w} + mb = \mathbf{1}^\top\mathbf{y}$$

$$\text{that is} \quad \begin{bmatrix} \mathbf{X}^\top\mathbf{X} & \mathbf{X}^\top\mathbf{1} \\ \mathbf{1}^\top\mathbf{X} & m \end{bmatrix} \begin{bmatrix} \boldsymbol{w} \\ b \end{bmatrix} = \begin{bmatrix} \mathbf{X}^\top\mathbf{y} \\ \mathbf{1}^\top\mathbf{y} \end{bmatrix}$$

where $\mathbf{1} = (1, 1, \ldots, 1)^\top$, an $m \times 1$ vector of “ones”

A different approach: $k-$nearest neighbours

Let $N(\boldsymbol{x}; k)$ be the set of k nearest training inputs to $\boldsymbol{x}$ and

$$I_{\boldsymbol{x}} = \{i : \boldsymbol{x}_i \in N(\boldsymbol{x}; k)\}$$

the corresponding index set

$$f(\boldsymbol{x}) = \begin{cases} \texttt{red} & \text{if } |\{y_i = \text{red} : i \in I_{\boldsymbol{x}}\}| > |\{y_i = \text{green} : i \in I_{\boldsymbol{x}}\}| \\ \texttt{green} & \text{if } |\{y_i = \text{green} : i \in I_{\boldsymbol{x}}\}| > |\{y_i = \text{red} : i \in I_{\boldsymbol{x}}\}| \end{cases}$$

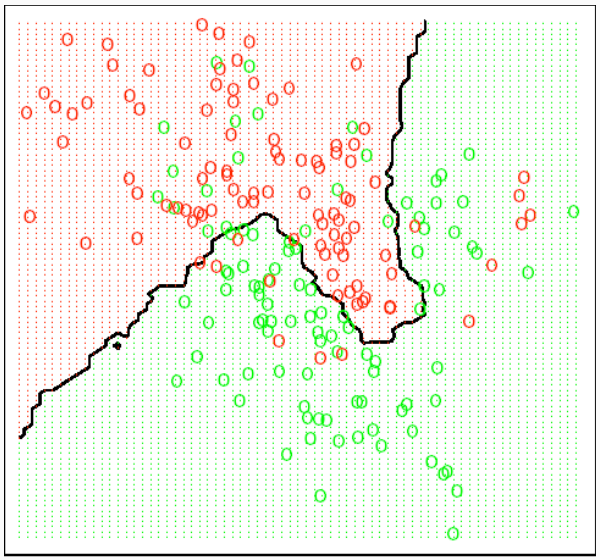
- Closeness is measured using a metric (eg, Euclidean dist.)
- Local rule (compute local majority vote)
- Decision boundary is non-linear

Note: for regression we set $f(\boldsymbol{x}) = \frac{1}{k} \sum_{i \in I_{\boldsymbol{x}}} y_i$ (a "local mean")

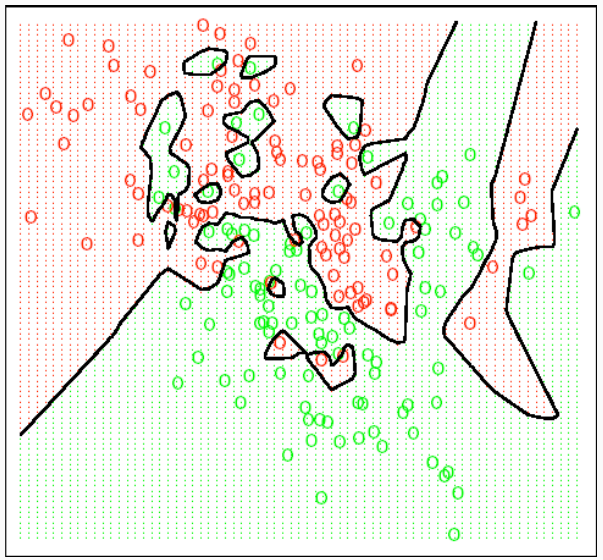
$k-$NN: the effect of k

- The smaller k the more irregular the decision boundary

$k = 15$



$k = 1$



- How to choose k? later...

Perspectives on supervised learning

Overview

We consider three influential ideas that underpin SL.

1. What is an optimal predictor? The Bayes estimator.
2. The bias and variance of a learning algorithm.
3. The non-existence of an optimal learning algorithm (without assumptions). NFL theorems.

Optimal Supervised Learning

Model: We assume that the data is obtained by sampling **i.i.d.** from a **fixed but unknown** probability distribution $P(\boldsymbol{x}, y)$

Expected error (wrt to the *squared loss*):

$$\mathcal{E}(f) := \mathbf{E}\left[(y - f(\boldsymbol{x}))^2\right] = \int (y - f(\boldsymbol{x}))^2 dP(\boldsymbol{x}, y)$$

Our goal is to minimize $\mathcal{E}$

Optimal solution: $f^* := \operatorname{argmin}_f \mathcal{E}(f)$ (called *Bayes estimator*)

Problem A: in order to compute f^* we need to know P!

Note: for binary classification with $\mathcal{Y} = \{0, 1\}$ and $f : \mathcal{X} \to \mathcal{Y}$, $\mathcal{E}(f)$ counts the average number of mistakes of f (aka expected misclassification error)

Bayes estimator for square loss

Let us compute the optimal solution f^* for regression $\mathcal{Y} = \mathbb{R}$.
Using the decomposition $P(y, \boldsymbol{x}) = P(y|\boldsymbol{x})P(\boldsymbol{x})$ we have

$$\mathcal{E}(f) = \int_{\mathcal{X}} \left\{ \int_{\mathcal{Y}} \left(y - f(\boldsymbol{x})\right)^2 dP(y|\boldsymbol{x}) \right\} dP(\boldsymbol{x})$$

Observe that f^* is

$$f^*(\boldsymbol{x}) = \int_{\mathcal{Y}} y dP(y|\boldsymbol{x})$$

Deriving the Bayes estimator for square loss

Deriving f^* in the discrete case,

$$\mathcal{E}(f) := \sum_{x \in X} \sum_{y \in Y} (y - f(x))^2 p(x, y)$$

and $\mathcal{E}(f)$ is the expected error of an arbitrary predictor f wrt the square loss and $p(x, y)$ is a probability mass function.

Separating

$$\mathcal{E}(f) = \sum_{x \in X} [\sum_{y \in Y} (y - f(x))^2 p(y|x)] p(x)$$

now let's find the value of $f^*(\cdot)$ for a given x. Define

$$\mathcal{E}(f(x)) := \sum_{y \in Y} (y - f(x))^2 p(y|x)$$

which denotes the expected error of f at x.

Derivation – continued (1)

Observe that,

$$\mathcal{E}(f) = \sum_{x \in X} \mathcal{E}(f(x))p(x)$$

i.e., the expected error of f is just the sum of expected errors from each 'x' weighted by the probability of each 'x'.

Let's solve for the value of f^* at x' by taking the derivative of $\mathcal{E}(f)$ wrt $f(x')$.

$$\begin{aligned}
\frac{\partial \mathcal{E}(f)}{\partial f(x')} &= \sum_{x \in X} \frac{\partial [\mathcal{E}(f(x))p(x)]}{\partial f(x')} \\
&= \frac{\partial [\mathcal{E}(f(x'))p(x')]}{\partial f(x')} + \cancel{\sum_{x \neq x'} \frac{\partial [\mathcal{E}(f(x))p(x)]}{\partial f(x')}} \\
&= \frac{\partial [\sum_{y \in Y} (y - f(x'))^2 p(y|x')p(x')]}{\partial f(x')}
\end{aligned}$$

Derivation – continued (2)

Set $z := f(x')$ and rewriting gives

$$\frac{\partial \mathcal{E}(f)}{\partial z} = \frac{\partial [\sum_{y \in Y} (y - z)^2 p(y|x') p(x')]}{\partial z}$$
$$= -2 \sum_{y \in Y} (y - z) p(y|x') p(x')$$

Setting equal to zero and solving,

$$0 = \left(\sum_{y \in Y} y p(y|x') - \sum_{y \in Y} z p(y|x') \right) \cancel{p(x')} = \sum_{y \in Y} y p(y|x') - z$$

which implies

$$z = \sum_{y \in Y} y p(y|x')$$

and hence since x' was generic

$$f^*(x) = \sum_{y \in Y} y p(y|x) = E[y|x] \,.$$

Bias and Variance of a learning algorithm

- We now additionally assume there exists some underlying function F such that

$$y = F(x) + \epsilon$$

  where ϵ is white noise, i.e., $E[\epsilon] = 0$ and finite variance.
- Thus the optimal prediction is $f^*(x) := E[y|x] = F(x)$ with square loss.
- We would like to understand the expected error by an arbitrary learner $A_{\mathcal{S}}(x)$ (we now drop the $\mathcal{S}$ for convenience).
- Our goal will be to understand the expected error at x'

$$\mathcal{E}(A(x')) = E[(y' - A(x'))^2]$$

  where y' is a sample from the marginal $P(y|x')$.

Useful Lemma and Corollary

Lemma

$$E[(Z - E[Z])^2] = E[Z^2] - E[Z]^2$$

Proof

$$E[(Z - E[Z])^2] = E[Z^2 - 2ZE[Z] + E[Z]^2]$$
$$E[(Z - E[Z])^2] = E[Z^2] - 2E[Z]^2 + E[Z]^2$$
$$= E[Z^2] - E[Z]^2$$

Corollary

$$E[Z^2] = E[(Z - E[Z])^2] + E[Z]^2$$

Decomposing $\mathcal{E}(A(x'))$

$$
\begin{aligned}
E[(y' - A(x'))^2] &= E[(y')^2 - 2y'A(x') + A(x')^2] \\
&= E[(y' - f^*(x'))^2] + f^*(x')^2 + \\
&\quad - 2f^*(x')E[A(x')] + \\
&\quad E[(A(x') - E[A(x')])^2] + E[A(x')]^2 \\
&= E[(y' - f^*(x'))^2] + \qquad \text{[Bayes error]} \\
&\quad (f^*(x') - E[A(x')])^2 + \quad \text{[bias}^2\text{]} \\
&\quad E[(A(x') - E[A(x')])^2] \quad \text{[variance]}
\end{aligned}
$$

- Bayes error : $E[(y' - f^*(x'))^2]$ is the irreducible noise.
- Bias : $f^*(x') - E[A(x')]$
  describes the discrepancy between the algorithm and "truth" .
- Variance : $E[(A(x') - E[A(x')])^2]$
  captures the variance of the algorithm between training sets

Subtlety: There are two *independent* random quantities. $A(\cdot)$ depends on the random draw of the training sequence and y' depends on the draw on from the marginal $p(y|x')$.

Bias and Variance Dilemma

- The bias and variance tend to trade off against one another
- Many parameters better flexibility to fit the data thus low bias but high variance
- Few parameters give high bias but the fit between different data sets will not change much thus low variance
- Caveat: this exact decomposition only holds for the square loss.

Optimal Algorithms and No Free Lunch Theorems

- Is there an optimal machine learning algorithm?
- I.e., an algorithm that does almost as well as the bayes estimator.
- There are a variety of such (NFL) results showing that no such algorithm exists.
- We give an example NFL Theorem in classification setting

Bayes estimator for classification

More generally the *Bayes classifier* (estimator) is the minimiser of the expected loss

- for C-class classification, f^* (called the Bayes classifier) is

$$f^*(\boldsymbol{x}) = \underset{c \in \{1,\ldots,C\}}{\operatorname{argmax}} \; P(Y = c|\boldsymbol{x})$$

  where the loss is 0 if we predict correctly and 1 otherwise.
- The *Bayes error rate* (optimal) is then

$$\int (1 - P(Y = f^*(\boldsymbol{x})|\boldsymbol{x}))dP(\boldsymbol{x})$$

Challenge: What is the Bayes estimator of

$$\mathcal{E}(f) := \sum_{x \in X} \sum_{y \in Y} |y - f(x)| p(x, y)$$

An NFL theorem for classification

Theorem

Let $A_{\mathcal{S}}$ be any learning algorithm for binary classification $\mathcal{Y} = \{0, 1\}$ over the domain $\mathcal{X}$. Let $m < |\mathcal{X}|/2$ then there exists some distribution P over $\mathcal{X} \times \{0, 1\}$ such that,

1. There exists a function $f : \mathcal{X} \to \{0, 1\}$ the Bayes error is 0.
2. With probability of at least $1/7$ with respect to a random draw $\mathcal{S}$ of m examples from P and a draw of a $m + 1$st example (x', y') we have that

$$\text{Prob}[A_{\mathcal{S}}(x') \neq y'] \geq 1/8$$

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Proof? Exercise!

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Proof? Exercise!

(No, seriously)

Asymptotic Optimality of k-NN

Revisiting k-NN

k-NN attempts approximate $P(Y = c|\boldsymbol{x})$ as $\frac{|\{i:y_i=c,i\in I_x\}|}{k}$

- Expectation is replaced by averaging over sample data
- Conditioning at $\boldsymbol{x}$ is relaxed to conditioning on some region close to $\boldsymbol{x}$

As the number of samples goes to infinity ($m \to \infty$) 1-NN and k-NN become “good” estimators.

1-NN is near asymptotically optimal

Theorem

As the number samples goes to infinity the error rate is no more than twice the Bayes error rate.

Proof Sketch

Abbreviate notation $P(c|\boldsymbol{x}) := P(Y = c|\boldsymbol{x})$.

The expected (Bayes) error of the Bayes classifer (at x) is

$$1 - \max_{c \in \{1,\ldots,C\}} P(c|\boldsymbol{x})$$

and the expected rate of 1-NN (at x) is

$$\sum_{c=1}^{C} P(c|\boldsymbol{x}_{nn})[1 - P(c|\boldsymbol{x})] \,.$$

Proof Sketch – continued

Proof Sketch

Observe that as the number samples goes to infinity, $m \to \infty$,

$$P(c|\boldsymbol{x}_{nn}) \approx P(c|\boldsymbol{x}) \qquad \text{(under some regularity assumption)}$$

thus the expected rate of 1-NN (at x) is

$$\sum_{c=1}^{C} P(c|\boldsymbol{x})[1 - P(c|\boldsymbol{x})] \,.$$

We need to show

$$\sum_{c=1}^{C} P(c|\boldsymbol{x})[1 - P(c|\boldsymbol{x})] \leq 2[1 - \max_{c \in \{1,\ldots,C\}} P(c|\boldsymbol{x})]$$

Proof Sketch – continued

Let $c^* = \text{argmax}_{c \in \{1,\ldots,C\}} P(c|\boldsymbol{x})$ and $p^* = P(c^*|\boldsymbol{x})$. Observe that

$$\begin{aligned}\sum_{c=1}^{C} P(c|\boldsymbol{x})[1 - P(c|\boldsymbol{x})] &= \sum_{c \neq c^*}^{C} P(c|\boldsymbol{x})[1 - P(c|\boldsymbol{x})] + p^*(1 - p^*) \\ &\leq (C-1)\frac{1-p^*}{C-1}[1 - \frac{1-p^*}{C-1}] + p^*(1-p^*) \\ &= (1-p^*)[1 - \frac{1-p^*}{C-1} + p^*]\end{aligned}$$

Where the second line follows since the sum is maximised when all "$P(c|\boldsymbol{x})$" have the same value (exercise!). And since $p^* < 1$ we are done. □

k-NN is asymptotically optimal

One can show that $\mathcal{E}(k(m) - NN) \to \mathcal{E}(f^*)$ as $m \to \infty$ provided that:

1. $k(m) \to \infty$
2. $\frac{k(m)}{m} \to 0$

Weakness: the rate of convergence depends exponentially on the input dimension. An example of the **curse of dimensionality**.

Reference for 1-NN near optimality
Cover & Hart : *Nearest Neighbor Pattern Classification*, 1967

Curse of dimensionality

1. "Curse of dimensionality" is an observation that many methods suffer as the dimensionality of data increases.
2. The intuition is that since volume increases *exponentially* with the dimension then the data required to "cover" the space to perform estimates also increase exponentially.
3. E.g., consider a d-dimensional unit cube versus the 1/2-unit cube. the ratios of their volumes is $\frac{1}{2}^d$.

- Potential "solutions" include limiting the number of hypotheses (functions) – i.e., introducing a *hypothesis space*. Alternately associating a "complexity" with each hypothesis and then "prefer" simpler hypothesis.

Linear regression vs. $k-$NN (informal)

- Parametric vs. non-parametric
- Global vs. local
- Linear vs. non-linear
- Bias / variance considerations:
  - LR relies heavily on linear assumption (may have large bias) k-NN does not
  - LR is stable (solution does not change much if data are perturbed) 1-NN isn't!
- $k-$NN sensitive to input dimension d: if d is high, the inputs tends to be far away from each other!

Hypothesis Space

Solving the "Problem A"

$P(\boldsymbol{x}, y)$ is unknown $\Rightarrow$ cannot compute $f^* = \operatorname{argmin}_f \mathcal{E}(f)$

We are only given a sample (training set) from P

A natural approach: we approximate the expected error $\mathcal{E}(f)$ by the empirical error

$$\mathcal{E}_{\text{emp}}(\mathcal{S}, f) = \frac{1}{m} \sum_{i=1}^{m} (y_i - f(\boldsymbol{x}_i))^2$$

Problem B: If we minimize $\mathcal{E}_{\text{emp}}$ over all possible functions, we can always find a function with zero empirical error! (if the Bayes error is zero).

Why is this a problem?

Solving the "Problem B"

A Proposed solution: we introduce a restricted space of functions $\mathcal{H}$ called the **hypothesis space**

We minimize $\mathcal{E}_{\text{emp}}(\mathcal{S}, f)$ within $\mathcal{H}$. That is, our learning algorithm is:

$$f_S = \text{argmin}_{f \in \mathcal{H}} \mathcal{E}_{\text{emp}}(\mathcal{S}, f)$$

This approach is usually called **empirical error (risk) minimization**

For example (Least Squares) :

$$\mathcal{H} = \{f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} : \boldsymbol{w} \in \mathbb{R}^n\}$$

Problem C: How do we choose a space $\mathcal{H}$ (discuss later)?

Choosing a Hypothesis Space (returning to prob. “C”)

Given the training data $y_i = f^*(\boldsymbol{x}_i) + \epsilon_i$, the goal is to compute an “approximation” of f^*.

We look for an approximant of f^* within a prescribed hypothesis space $\mathcal{H}$

- Unless prior knowledge is available on f^* (eg, f^* is linear) we cannot expect $f^* \in \mathcal{H}$
- Choosing $\mathcal{H}$ “very large” leads to overfitting! (we’ll see an example of this in a moment)

Summary

- Data S sampled i.i.d from P (fixed but unknown)
- f^* is what we want, f_S is what we get
- Different approaches to attempt to estimate/approximate f^*:
  - Minimize $\mathcal{E}_{\text{emp}}$ in some restricted space of functions (eg, linear)
  - Compute local approximation of f^* (k-NN)
  - Estimate P and then use Bayes rule...

Model Selection

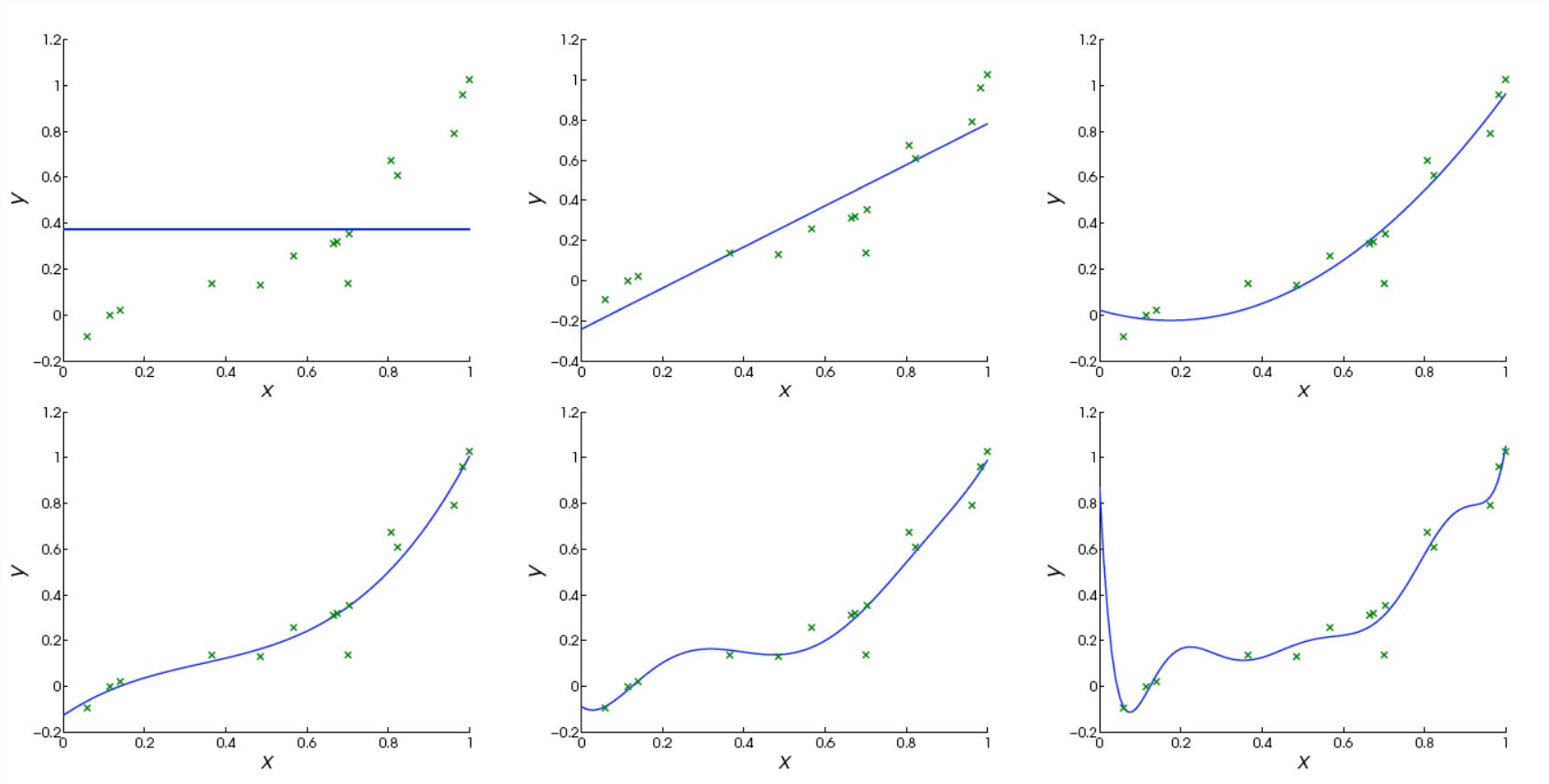
Polynomial fitting

As an example of hypothesis spaces of increasing "complexity" consider regression in one dimension

$$
\begin{aligned}
H_0 &= \left\{ f(x) = b : b \in \mathbb{R} \right\} \\
H_1 &= \left\{ f(x) = ax + b : a, b \in \mathbb{R} \right\} \\
\\
H_2 &= \left\{ f(x) = a_1 x + a_2 x^2 + b : a_1, a_2, b \in \mathbb{R} \right\} \\
&\vdots \\
H_n &= \left\{ f(x) = \sum_{\ell=1}^{n} a_\ell x^\ell + b : a_1, \ldots, a_n, b \in \mathbb{R} \right\}
\end{aligned}
$$

Consider minimizing the empirical error in $\mathcal{H}_r$ ($r =$ "polynomial degree")

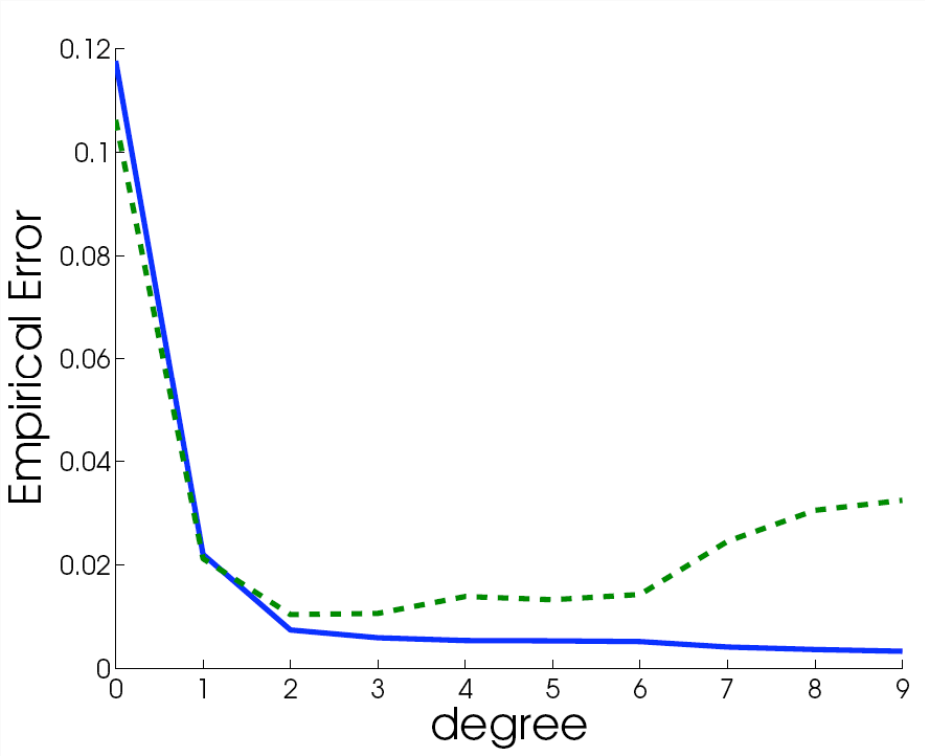
Polynomial fitting (simulation)



$r = 0, 1, 2, 3, 4, 5$. As r increases the fit to the data improves (empirical error decreases)

Overfitting vs. Underfitting

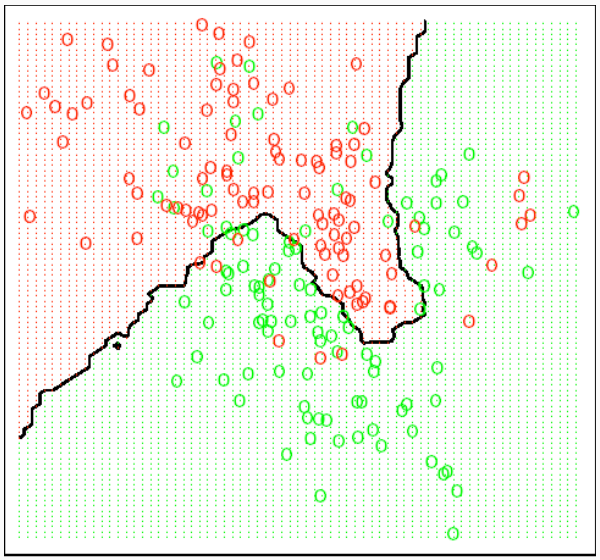
- Compare the empirical error (solid line) with expected error (dashed line)
  - r small: underfitting
  - r large: overfitting
- The larger r the lower the empirical error of f_S! $\Rightarrow$ We cannot rely on the training error!



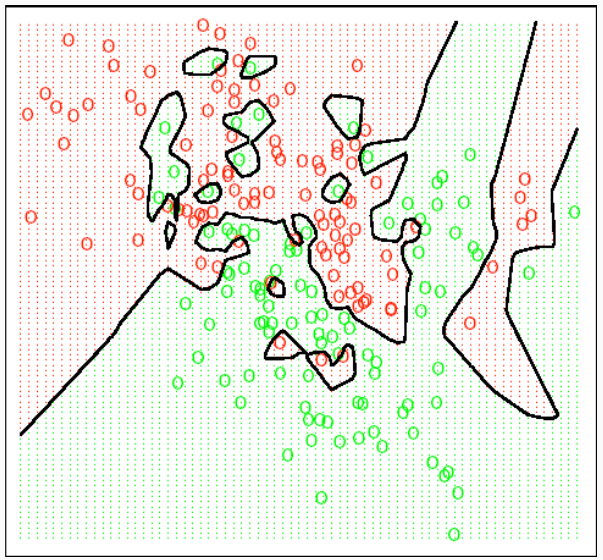
$k-$NN: the effect of k

- The smaller k the more irregular the decision boundary

$k = 15$



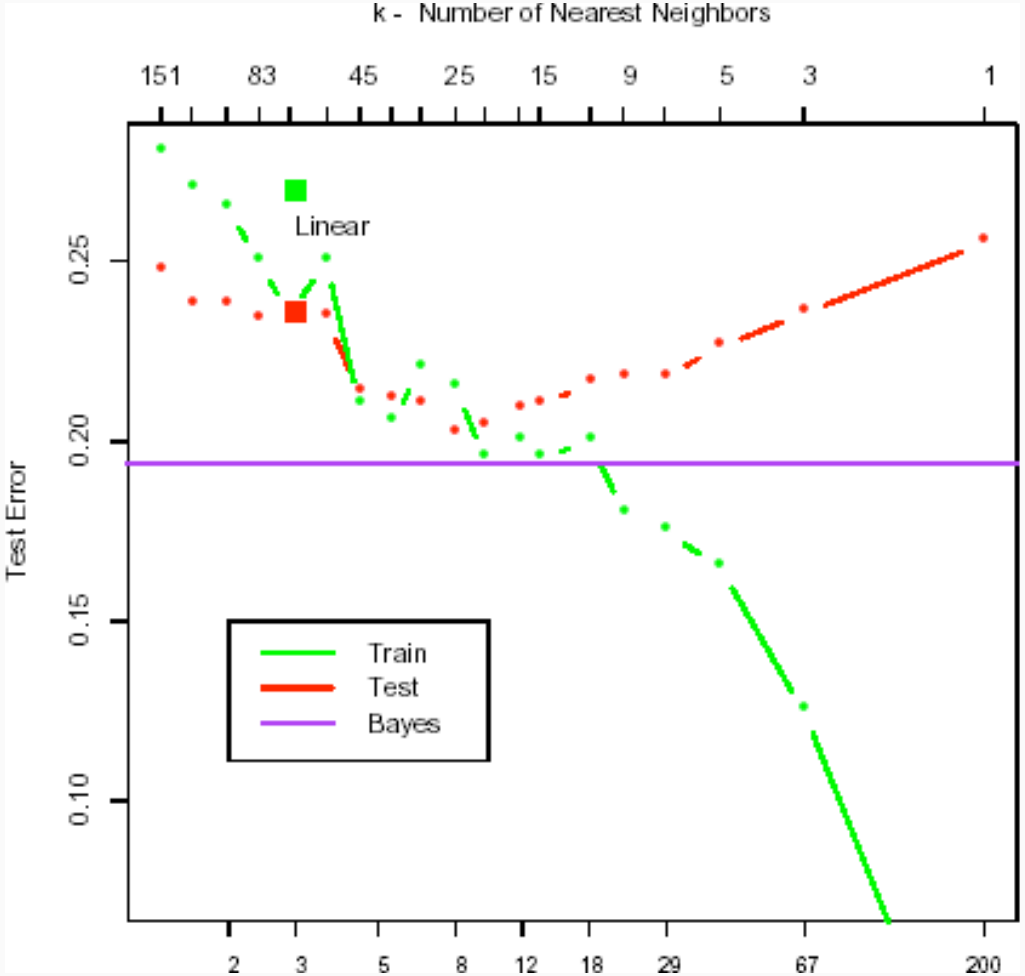
$k = 1$



- How to choose k? later...

$k-$NN: the effect of k

$\frac{m}{k}$ large: overfitting versus $\frac{m}{k}$ small: underfitting



Model Selection

1. How to choose k in k-NN?
2. How to choose the degree r for polynomial regression?
3. The simplest approach is to use part of the training data (say 2/3) for training and the rest as a validation set for each $\mathcal{H}_r$
4. Another approach is $K-$fold cross-validation – see next slide
5. Then choose the "best" r relative to the error(s) on the validation set
6. We will return to model selection later in the course

Cross-validation

1. we split the data in K parts (of roughly equal sizes)
2. repeatedly train on $K - 1$ parts and test on the part "left out"
3. average the errors of K "validation" sets to give so-called cross-validation error
4. smaller K is less expensive but poorer estimate as size of training set is smaller and random fluctuations larger

For a dataset of size m, m -fold cross-validation is referred to as leave-one-out (LOO) testing

Cross-validation comments

- Cross validation is good in “practice.”
- There are a variety of theoretical-based approaches (not covered today)
- Examples
    1. “Bayesian” model selection via the “evidence”
    2. Structural Risk Mininimization

Other learning paradigms

- **Online learning:** we observe the data sequentially and we make a prediction and update are learner after every datum.
- **Active learning:** we are given many inputs and we can choose which ones to request a label.
- **Unsupervised learning:** we have only input examples. Here we may want to find data clusters, estimate the probability density of the data, find important features/variable (dimensionality reduction problem), detect anomalies, etc.
- **Semi-supervised learning:** the ‘learning environment” may give us access to many input examples but only few of them are labeled.
- **Reinforcement learning:** Similar to online learning where data is received sequentially but feedback is often delayed.

Suggested Readings

- Elements of Statistical Learning, 2ed, Chapter 2 : spans most of material of this lecture, with the following exceptions
- Cover & Hart : *Nearest Neighbor Pattern Classification*, 1967 : for Asymptotic Optimality of k-NN
- *Understanding Machine Learning from Theory to Algorithms*, Chapter 5.1 : For the NFL Theorem. See section 19.2.2 for a discussion of the curse of dimensionality wrt $K - nn$.

Going Deeper ...

- *Reconciling modern machine learning practice and the bias-variance trade-off.* Suggests that the classic U-shaped curve (see page 67) can be replaced by a double U, in a number of scenarios.
- *An adaptive nearest neighbor rule for classification.* Gives bounds for a k-NN variant that adapts k locally for each neighbourhood.

Problems – 1

1. True or False?

   "For the K-nearest neighbour algorithm, larger K values will tend to lead to overfitting."

   Explain your answer.

2. - First, give Cover's bound on the Bayes error of the 1-nearest neighbour algorithm as the number of examples goes to infinity.
   - Second, give an example where the 1-nearest neighbour algorithm achieves the Bayes error as the number of examples goes to infinity, explain your reasoning.

3. How can we choose k to ensure that the k-NN makes an unambiguous decision in the two-class case provided the test point is not equidistant to any pair of points in the training set? What values of k give an unambiguous decision under similar assumptions for the 3-class case?

Problems – 2

1. One of the drawbacks of the nearest-neighbour algorithm is that we must retain all of the training data. Describe a situation where a training point can be removed without affecting the resulting 1-NN classification for any test point in the input space.
2. In linear regression it is common to transform the training data

   $$(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)$$

   to

   $$((\boldsymbol{x}_1, 1), y_1), \ldots, ((\boldsymbol{x}_m, 1), y_m)$$

   i.e., we add an additional component to each input vector and set it to 1. What is the motivation for this procedure?
3. Given we have a dataset $\{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_m, y_m)\}$ where $\boldsymbol{x} \in \mathbb{R}^n$ and $y \in \{1, 2, \ldots, K\}$. Thus the inputs are real vectors and the labels denote one of K classes. How can linear regression (least squares), be used or adapted to tackle such a multi-class classification problem?