Data Science for Geosciences

Introduction

2017-18

Organization

Volume

- 5 × 3h lecture and pratices sessions
- 5 × 3h Lab/project sessions

Objectives

- model/algorithm analysis for supervised learning
- assess the quality of predictions and inferences
- application of these algorithms on different datasets from geosciences : ecology, geography, ocean-atmosphere, astrophysics, etc. . .

Schedule

	Monday	Tuesday	Wednesday	Thursday	Friday
9h-12h	General introduction	Regression	Model selection	Deep learning	Project
14h-17h	Project	Classification	Project	Project	Project

Remarks

- ice-breaker on Monday night

Reference books

Trevor Hastie, Robert Tibshirani et Jerome Friedman (2009)
The Elements of Statistical Learning (2nd Edition)
Springer Series in Statistics

Christopher M. Bishop (2007)
Pattern Recognition and Machine Learning *Springer*

Richard O. Duda, Peter E. Hart et David G. Stork (2001)
Pattern classification (2nd edition) *Wiley*

Supplementary materials, datasets, online courses, ...

`http://www-stat.stanford.edu/~tibs/ElemStatLearn/`

`http://research.microsoft.com/en-us/um/people/cmbishop/prml/`

`https://www.coursera.org/course/ml` *very popular MOOC (Andrew Ng)*

`https://work.caltech.edu/telecourse.html` *more involved MOOC (Y. Abu-Mostafa)*

`https://dsg2018.wordpress.com` *webpage for this course*

Data Science

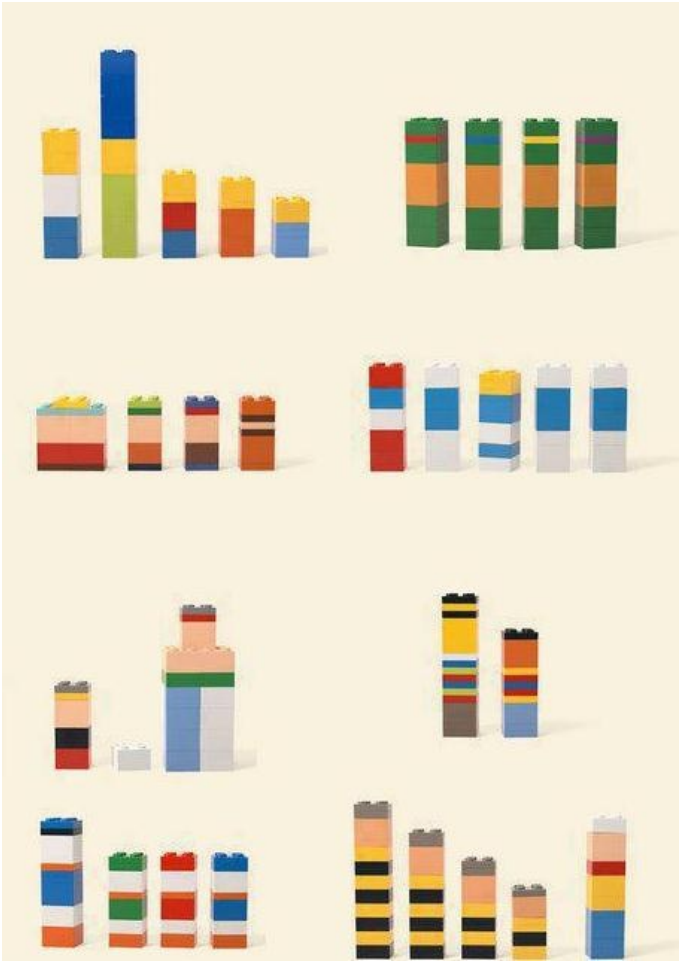
How to extract knowledge or insights from data ?

Learning problems are at the cross-section of several applied fields and science disciplines

- Machine learning arose as a subfield of Artificial Intelligence and Computer Science. Emphasis on large scale implementations and applications (algorithm centered)
- Statistical learning arose as a subfield of Statistics, Applied Maths, Signal Processing,... Emphasizes models and their interpretability (model centered)

☞ There is much overlap : Data Science

Learning problem



Definitions of Learning

Machine Learning in Computer Science

Tom Mitchell (The Discipline of Machine Learning, 2006)

A computer program CP is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E

Key points

- Experience E : data and statistics
- Performance measure P : soptimization
- tasks T : utility
  - automatic translation
  - playing Go
  - ... doing what human does

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Experience E : the data !

Type of data : qualitatives / ordinales / quantitatives variables

text	strings
speech	time series
images/videos	2/3d dependences
networks	graphs
games	interaction sequences
	...

Big data (volume, velocity, variety, veracity)

Data are available without having decided to collect them !

- importance of preprocessings (cleaning up, normalization, coding,...)
- importance of a good representation : from raw data to vectors

Objective and performance measures P

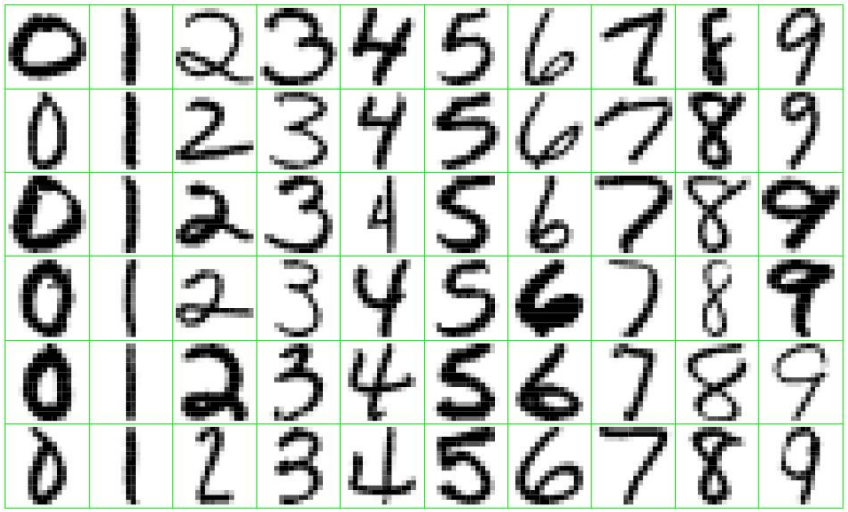
Generalize

- Perform well (minimize P) on new data (fresh data, i.e. unseen during learning)
- ☞ Derive good (P/error rate) prediction functions

Examples of Tasks

TODO : To be changed with project applications

Recognition of handwritten digits (US postal envelopes)



- ☞ Predict the class (0,...,9) of each sample from an image of 16×16 pixels, with a pixel intensity coded from 0 to 255
- ▶ Low error rate to avoid wrong allocations of mails !

Supervised classification

Examples of Tasks

TODO : To be changed with project applications

Spams Recognition

Spam

```
WINNING NOTIFICATION
We are pleased to inform you of the result
of the Lottery Winners International
programs held on the 30th january 2005.
[...]  You have been approved for a lump sum
pay out of 175,000.00 euros.
CONGRATULATIONS!!!
```

No Spam

```
Dear George,
Could you please send me the report #1248 on
the project advancement?
Thanks in advance.

Regards,
Cathia
```

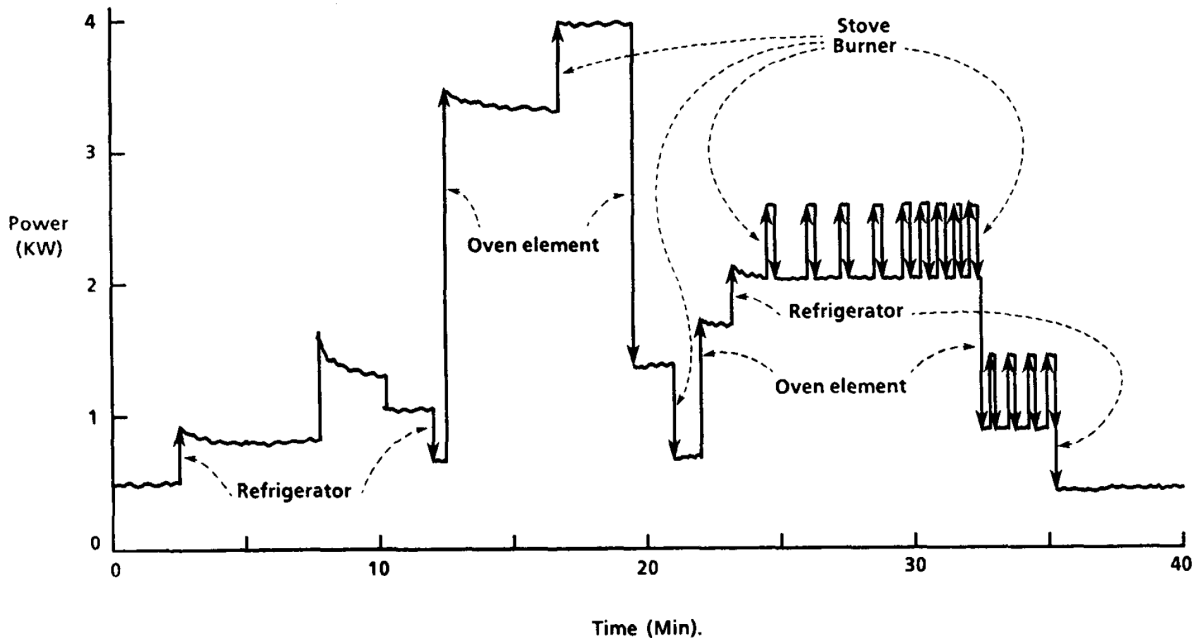
- ☞ Define a model to predict whether an email is spam or not
- ▶ Low error rate to avoid deleting useful messages, or filling the mailbox with useless emails

supervised classification

Examples of Tasks

TODO : To be changed with project applications

Disaggregation/Prediction of appliance's, or industrial, load



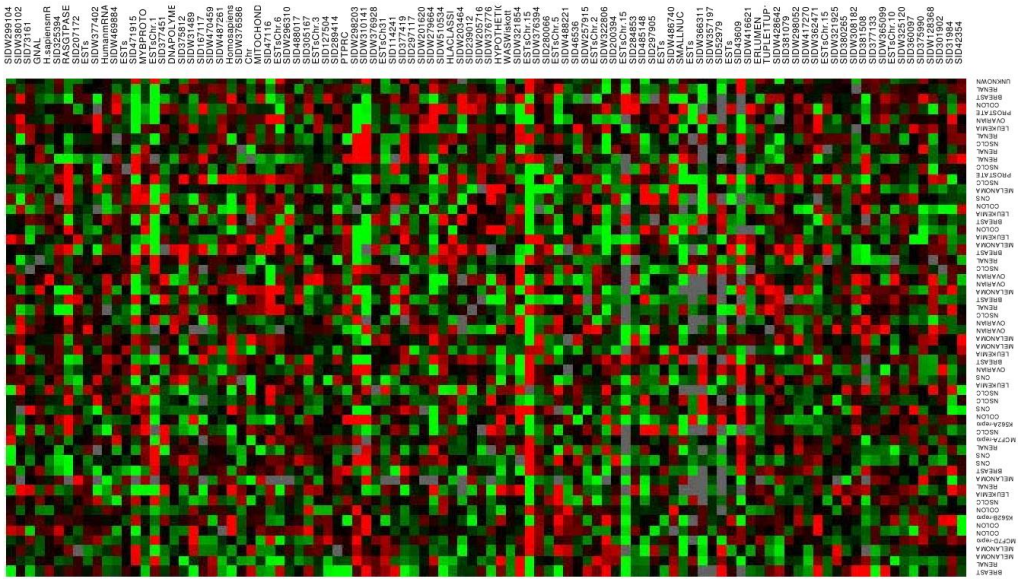
- Individual appliance recognition from load curves
- Predict the energy consumption

supervised or unsupervised classification

Examples of Tasks

TODO : To be changed with project applications

DNA-microarrays



- Genes expression dataset fore several thousand individual genes (columns) and tens of samples (rows)
- ☞ Classification of genes (resp. samples) with similar expression profiles across samples (resp. genes)

unsupervised classification

Definitions

Variable terminology

- observed data referred to as *input* variables, *predictors* or *features* ← usually denoted as X
- data to predict referred to as *output* variables, or *responses* ← usually denoted as Y

Type of prediction problem : regression vs classification

Depending on the type of the *output* variables

- when Y are quantitative data (continuous variables, e.g. electrical load curve values) ← regression
- when Y are categorical data (discrete qualitative variables, e.g. handwritten digits $Y \in \{0, \ldots, 9\}$) ← classification

Two very close problems

Prediction problem

Assumptions

- couples of input and output variables (X_i, Y_i) are i.i.d.
- input variables X_i are vectors in $\mathbb{R}^p$:

$$X_i = (X_{i,1}, \ldots, X_{i,p})^T \in \mathcal{X} \subset \mathbb{R}^p$$

- output variables Y_i take values :
  - in $\mathcal{Y} \subset \mathbb{R}$ (regression)
  - in a finite set $\mathcal{Y}$ (classification)

Prediction rule

function of prediction / rule of classification $\equiv$ function $f : \mathcal{X} \to \mathcal{Y}$ to get predictions

$$\widehat{Y} = f(X)$$

of new elements Y given X

Supervised or unsupervised learning

Training set $\equiv$ available sample $\mathcal{T}$ to learn the prediction rule f

For a sized n training set, different cases :

- Supervised learning : $\mathcal{T} \equiv ((X_1, Y_1), \ldots, (X_n, Y_n))$ input/output couples are available to learn the prediction rule f
- Unsupervised learning : $\mathcal{T} \equiv (X_1, \ldots, X_n)$ only the inputs are available
- Semi-supervised : mixed scenario (often encountered in practice, but less information than in the supervised case)

Academic example of binary classification

- Binary output variables : $Y_i \in \{0, 1\}$,
- Input variables $X_i \in \mathbb{R}^2$, for $i = 1, \ldots, N$

Example of a binary classification problem in $\mathbb{R}^2$*. The 2 classes are coded as a binary variable :* *ORANGE*=*1*, *BLUE*=*0*.

Simple linear model for classification

We seek a prediction model based on the linear regression of the outputs $Y \in \{0, 1\}$:

$$Y = \beta_1 X_1 + \beta_2 X_2 + \epsilon,$$

where $\boldsymbol{\beta} = (\beta_1, \beta_2)^T$ is a 2D unknown parameter vector

Learning problem $\Leftrightarrow$ Estimation of $\boldsymbol{\beta}$

Least Squares Estimator $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1, \hat{\beta}_2)^T$: minimize the training error rate (quadratic cost sense)

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{N} (Y_i - \beta_1 X_{i,1} - \beta_2 X_{i,2})^2$$

Classification rule based on least squares regression

$$f(X) = \begin{cases} 1 \text{ if } \widehat{Y} = \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 \geq 0.5, \\ 0 \text{ otherwise} \end{cases}$$

Simple linear model for classification (Cont'd)

Example of classification in $\mathbb{R}^2$*. The 2 classes are coded as a binary variable :* $ORANGE$*=1,* $BLUE$*=0. The line is the decision boundary* $z = \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 = 0.5$ *:* $BLUE$ *decision region below,* $ORANGE$ *one above*

'Black Box' method : k Nearest-Neighbors (k-NN)

The prediction model is directly defined, for $X = x$, as :

$$\widehat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i,$$

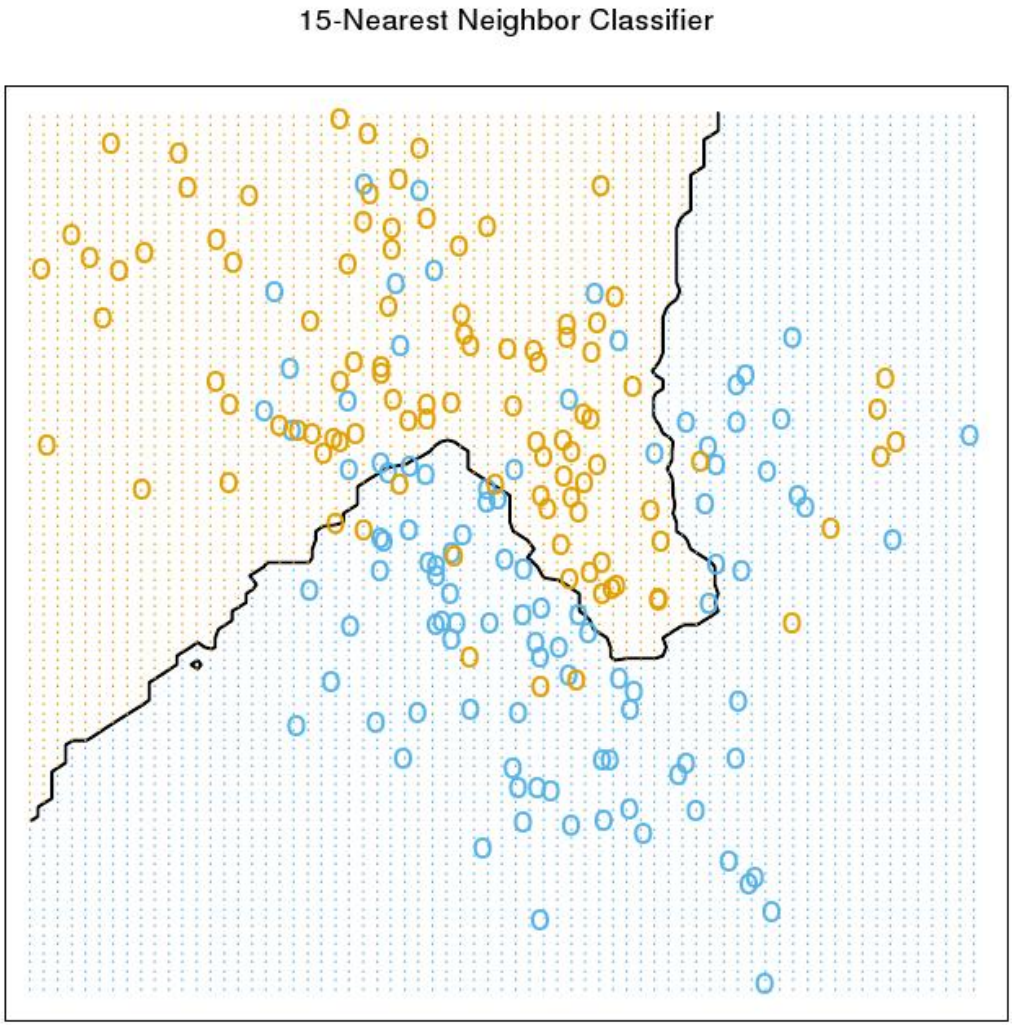
where $N_k(x)$ is the neighborhood of x defined by the k closest inputs X_i in the training sample.

Classification rule associated with k-NN

$$f(X) = \begin{cases} 1 \text{ if } \widehat{Y}(x) > \frac{1}{2}, \\ 0 \text{ otherwise} \end{cases}$$

$\Leftrightarrow$ majority vote among the k closest neighbors of the testing point x

K Nearest-Neighbors (Cont'd)



Model complexity

Most of methods have a complexity related to their *effective* number of parameters

Linear regression : model order p

E.g. dth degree polynomial regression : $p = d + 1$ parameters a_k s.t.

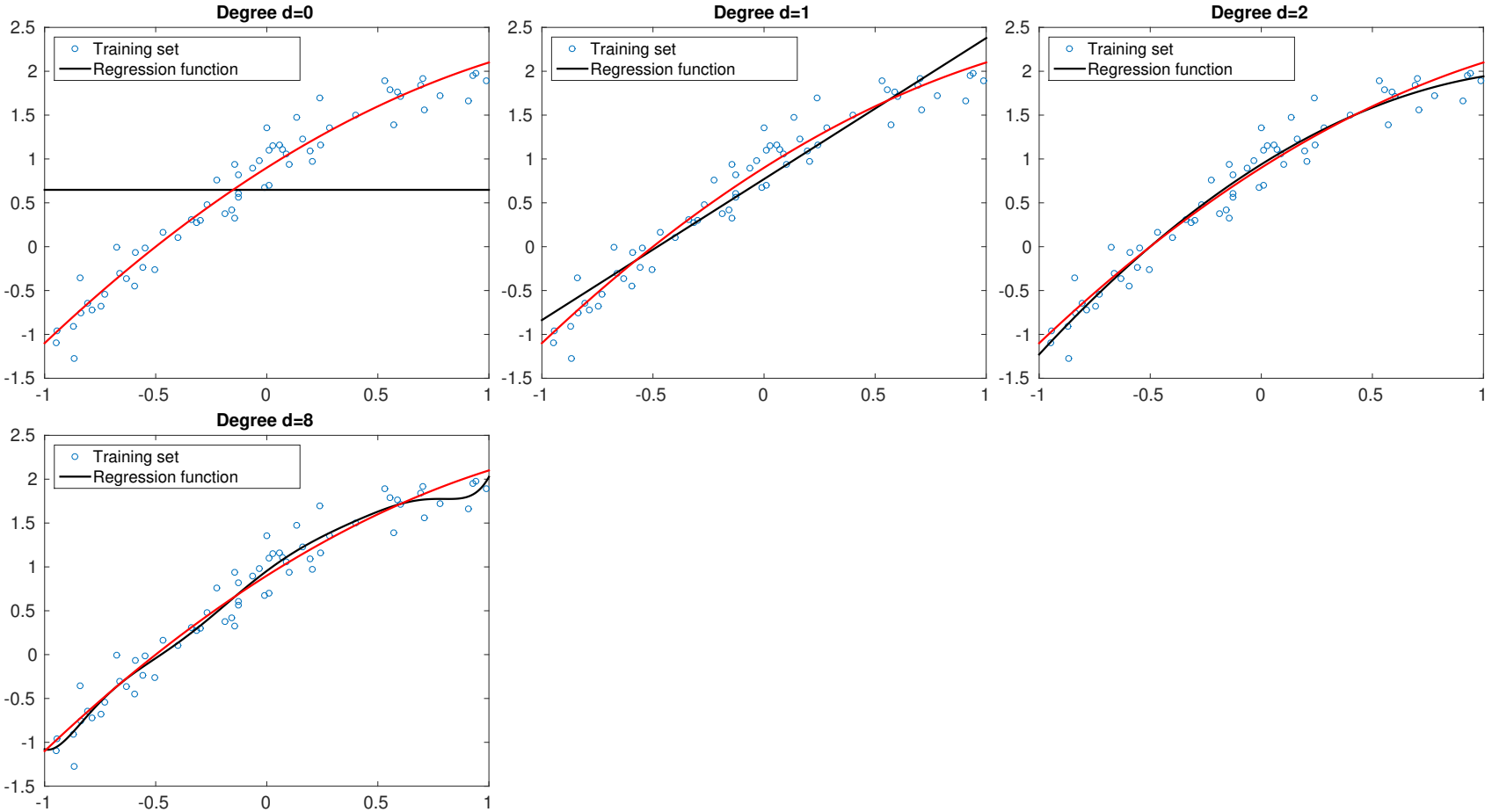
$$\begin{aligned} Y &= \sum_{k=0}^{d} a_k x^k + \epsilon, \\ &= \boldsymbol{X}_d \boldsymbol{a}_d + \epsilon, \end{aligned}$$

where

$$\begin{aligned} \boldsymbol{X}_d &= \left[x^0, x^1, \ldots, x^d \right], \\ \boldsymbol{a}_d &= \left[a_0, a_1, \ldots, a_d \right]^T. \end{aligned}$$

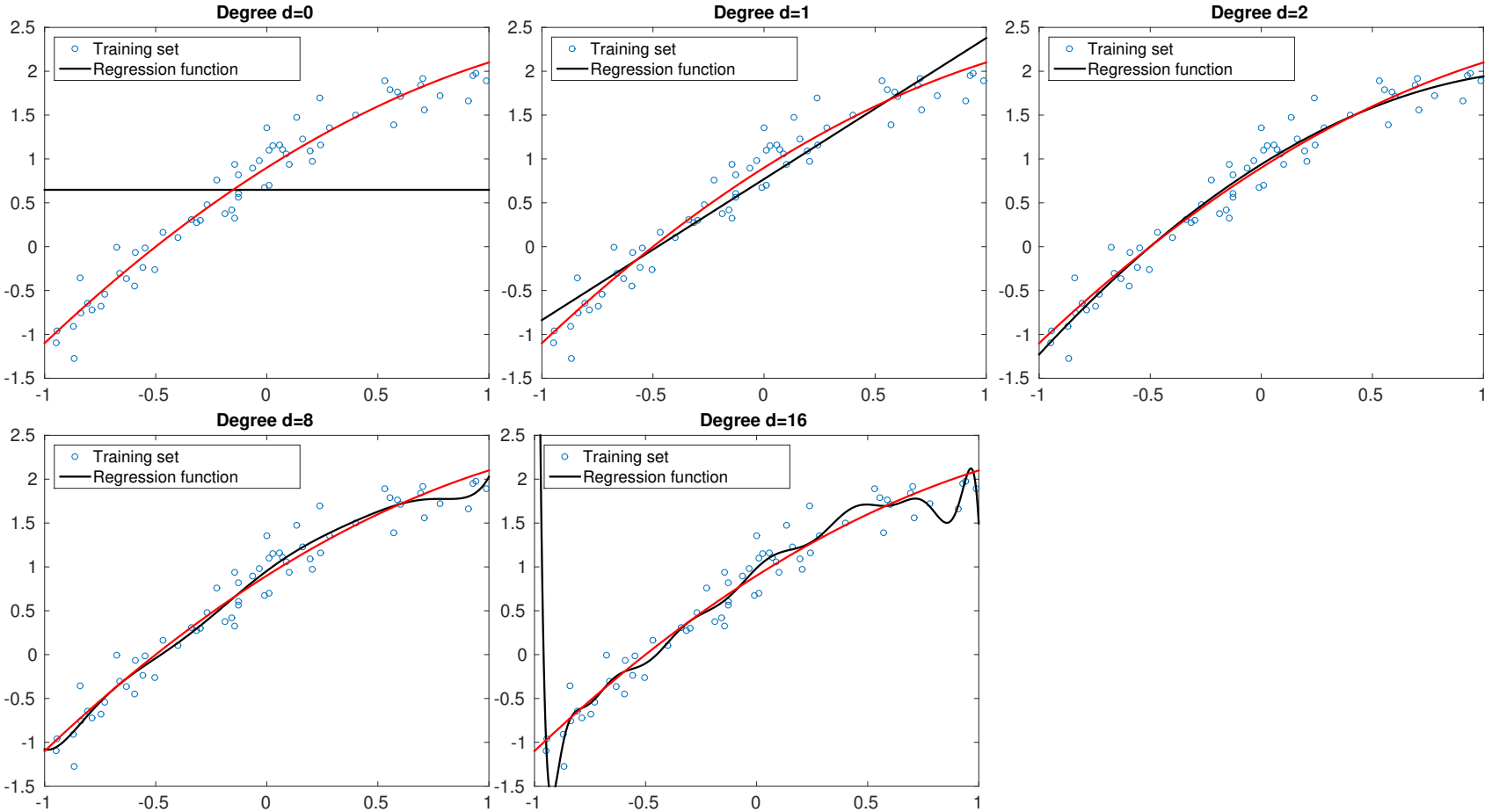
Linear regression : complexity vs stability

Polynomial degree d influence



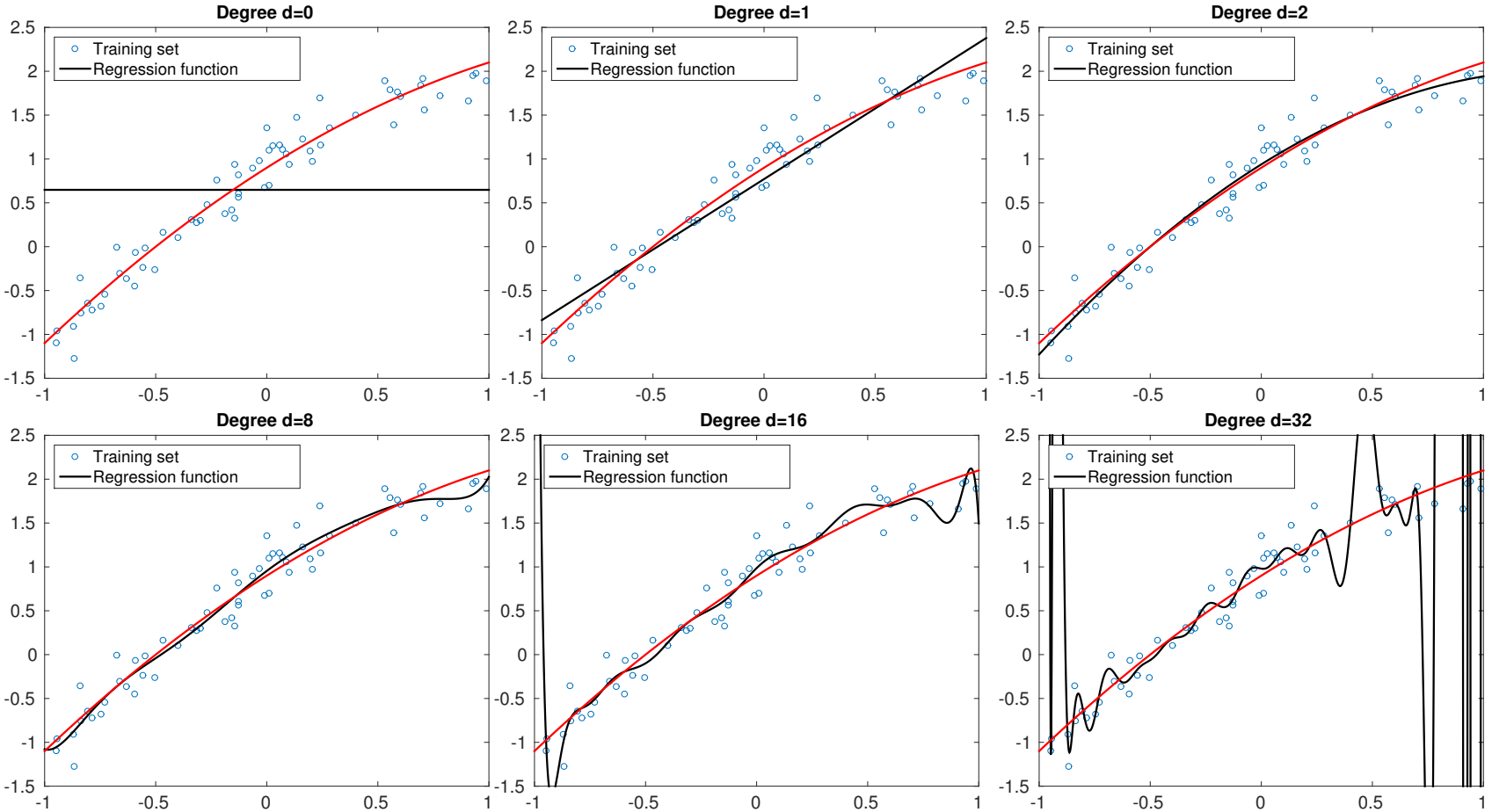
Linear regression : complexity vs stability

Polynomial degree d influence



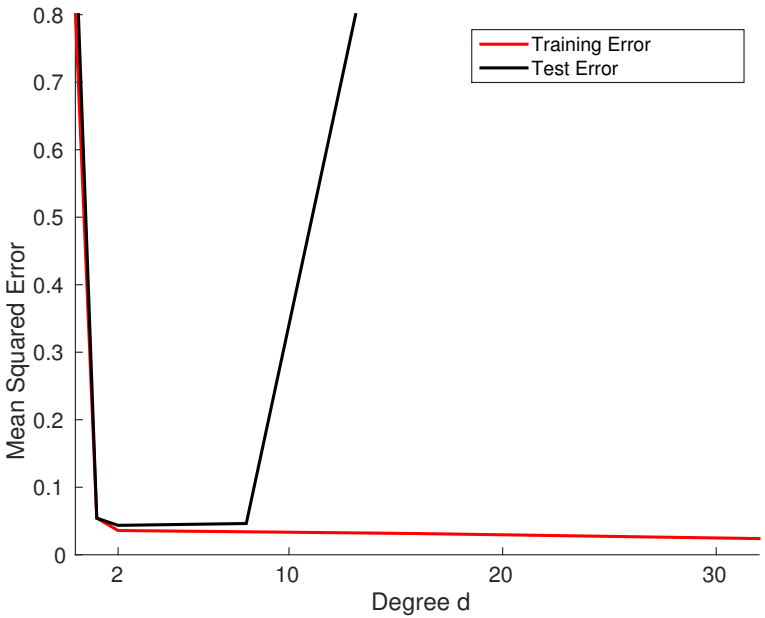
Linear regression : complexity vs stability

Polynomial degree d influence ← over-fitting



Linear Regression : Test error vs Train Error

Error rate vs polynomial order d



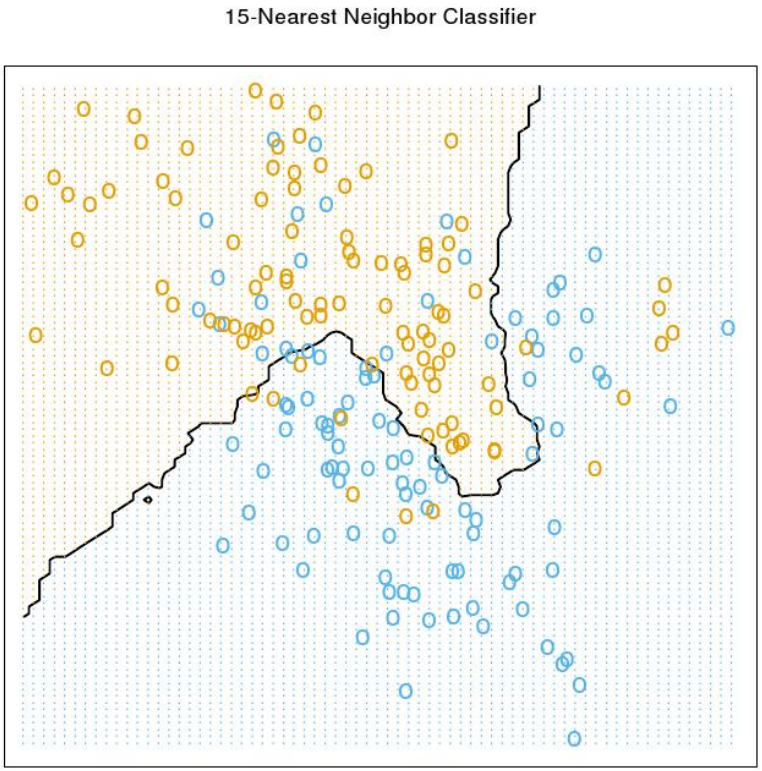
- True error rate (i.e. error rate for test data not used for learning) minimized when $d = 2$ ...
- ... true generative model : order $d = 2$ polynomial (+ white noise)

☞ Training error always decrease with the model complexity. Can't use alone to select the model !

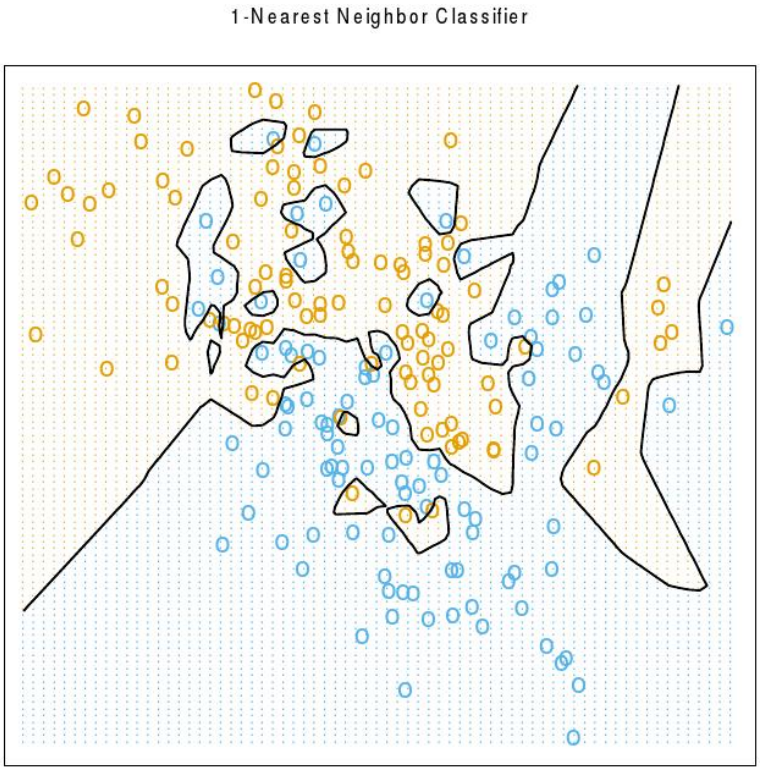
K Nearest-Neighbors

k-NN : complexity parameter k

The effective number of parameters expresses as $N_{\text{eff}} = \frac{N}{k}$, where N is the size of the training sample



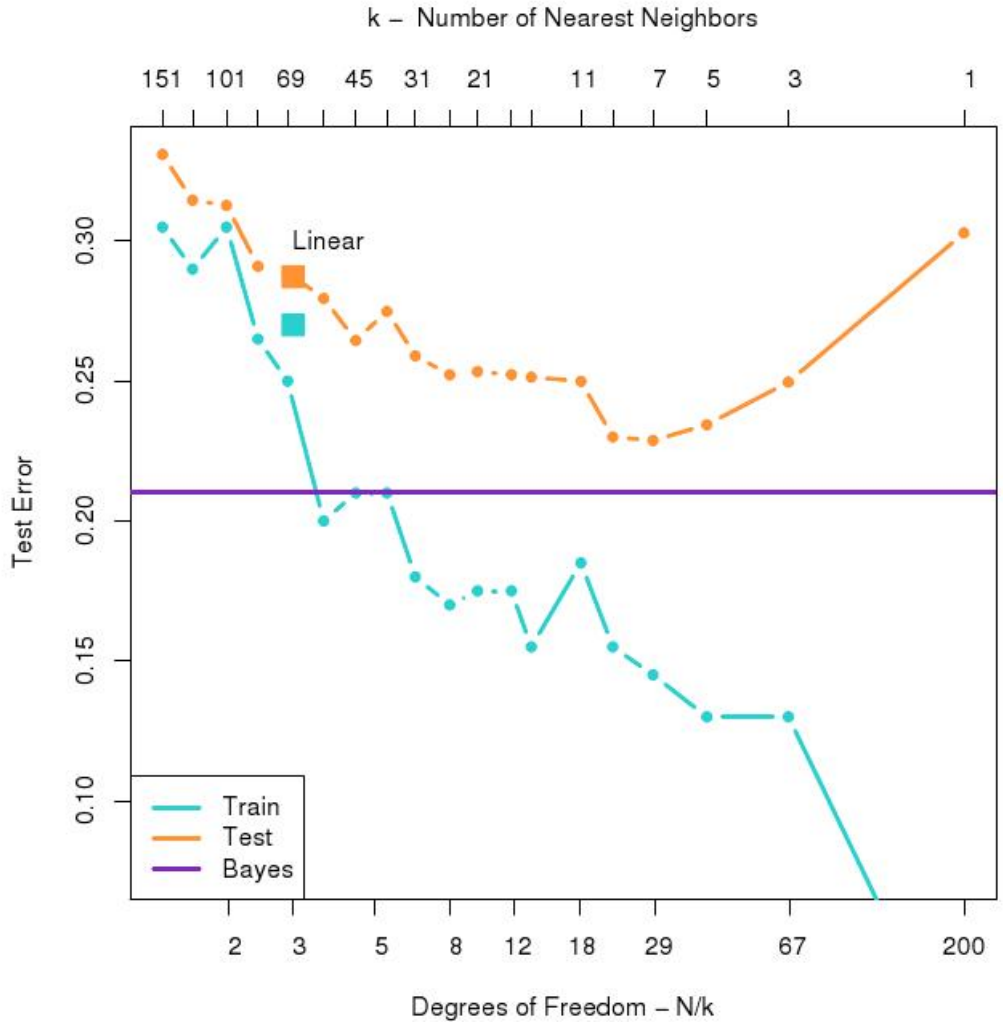
$k = 15,\ N_{\text{eff}} \approx 13$



$k = 1,\ N_{\text{eff}} \approx 200$

- $k = 1 \rightarrow$ training error is 0 !

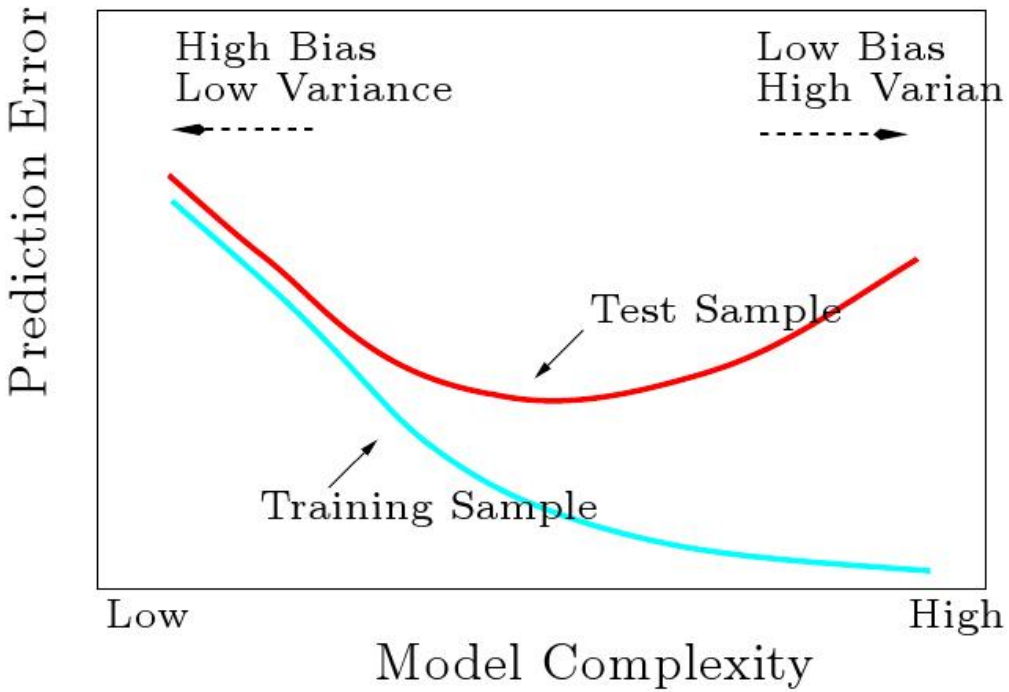
Model Selection



Model Selection (Cont'd)

Fundamental trade-off

- too simple model (high bias) → under-fitting
- too complex model (high variance) → over-fitting



Fundamental Bias-Variance trade-off

if the true model is

$$Y = f(X) + \epsilon,$$

then for any prediction rule $\widehat{f}(X)$, Mean Squared Error (MSE) expresses as

$$E\left[\left(Y - \widehat{f}(x)\right)^2\right] = \text{Var}\left[\widehat{f}(x)\right] + \text{Bias}\left[\widehat{f}(x)\right]^2 + \text{Var}\left[\epsilon\right]$$

- Var $[\epsilon]$ is the *irreducible* part
- as the flexibility of $\widehat{f}$ $\nearrow$, its variance $\nearrow$ and the bias $\searrow$

☞ overfitting/underfitting trade-off

The truth on the example dataset !

Generative model

- For $k = 1, \ldots, 10$, $m_k^1 \sim \mathcal{N}((0,1)^T, \boldsymbol{I})$ and $m_k^0 \sim \mathcal{N}((1,0)^T, \boldsymbol{I})$
- For $l = 1, \ldots, 100$, uniformly pick one m_k^1, then draw $x_l^1 \sim \mathcal{N}(m_k^1, \boldsymbol{I}/5)$
- Same for x_l^0 with the m_k^0 ($N = 200$ for the training sample size)