Statistical Learning

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Preliminary note

The material in these slides is strongly based on [1]. When other materials are used, they are cited accordingly.
Mathematical notation follows as good as it can a good practices proposal from the Beijing Academy of Artificial Intelligence.

What to expect?

In this session we will discuss:

- Modelling data.
- Models with independent and identically distributed (iid) data.
- The modelling dilemma.
- Loss function and risk.
- Polynomial regression.

How is data analyzed and used?

Statistical learning interpret the model and quantify the uncertainity of the data.

Machine learning (or *data mining*) making predictions using large scale data.

The goals of modelling data are:

- to predict data, based on existing one;
- to discover unusual or interesting patterns in data.

Types of machine learning

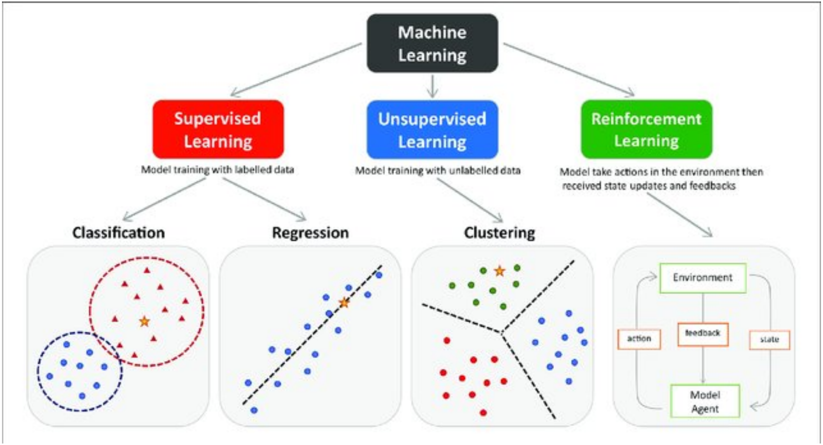


Figure 1: Different types of machine learning techniques[2]

Supervised vs unsupervised

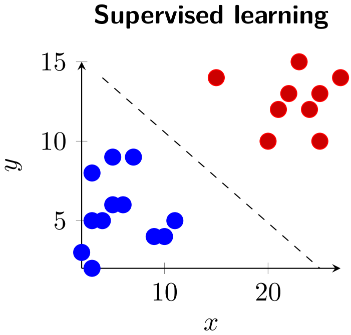


Figure 2: Supervised vs unsupervised ML

Example of modelling data I

Imagine an unsupervised learning problem, with data represented by a vector $\boldsymbol{x} = [x_1, \ldots, x_p]^\intercal$, a very general model is to assume that $\boldsymbol{x}$ is the outcome of a random vector $\boldsymbol{X} = [X_1, \ldots, X_p]^\intercal$ with some unknown pdf f.

The model can be refined by assuming a specific form of f.

Example of modelling data II

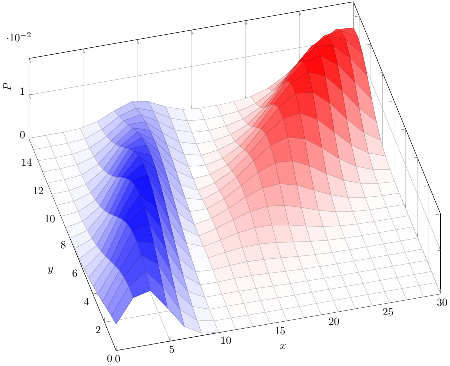
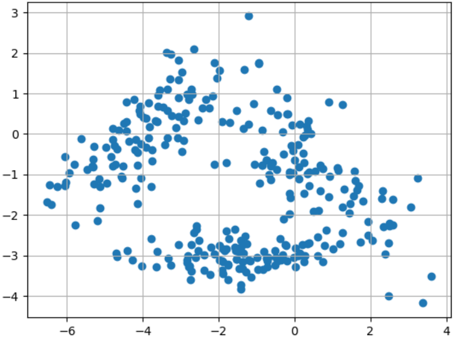


Figure 3: Some unknown pdf f from which data in Figure 3 was sampled.

Example of unsupervised modelling

Exercise 1 Unsupervised learning

Using the data in the file, try to find 3 clusters using the K-means method.



Tools to model data

Function approximation Model data with approximate and simple functions or maps.

Optimization Given a set of feasible mathematical models to the data, we may need to find the optimal one by fitting or callibrating a function to observed data.

Probability and Statistics Probability theory and statistical inference provides ways to quantify the uncertainity inherent in making predictions based on observed data.

iid data

If we are given a sequence of data vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_1$ one of the simplest possible models is to assume that the corresponding random vectors $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ are independent and identically distributed (iid). We express this as:

$$\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n \overset{iid}{\sim} f$$

meaning that the random vectors form an iid sample from a pdf f or sampling distribution *Dist*.
This is the same as saying that knowing about one variable does not provide information about another variable.

Independent data models

In independent data models, the joint density of the random vectors $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ is the *product* of the marginal ones:

$$f_{\boldsymbol{X_1},\ldots,\boldsymbol{X_n}}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = f(\boldsymbol{x}_1) \cdots f(\boldsymbol{x}_n)$$

The function $g(\boldsymbol{x})$, our "model" for $f(\boldsymbol{x})$, is usually specified up to a small number of parameters, corresponding to :

- $\mathcal{N}(\mu, \sigma^2)$
- $\mathrm{Bin}(n, p)$
- $\mathrm{Exp}(\lambda)$

The parameters are typically obtained from the data.

Modeling dilemma

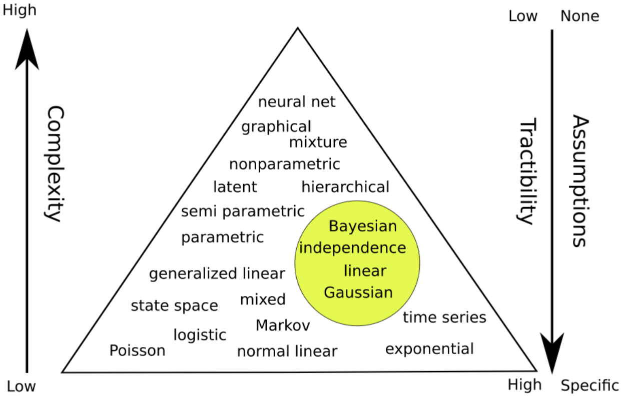


Figure 4: Complex models (very few of them) generally applicable but difficult to analyze. Simple models (a lot of options) very tractable but they do not describe well the data[1].

Tradeoff

There exists a tradeoff between model tractability and applicability, as seen in Figure 4. Coming back to the example in page 8, the *training set* $\tau = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is viewed as the outcome of n iid random variables $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ for some unknown pdf f.

Goal: to learn or estimate f from the finite training set.

Tradeoff vs risk

Imagine the **unsupervised learning** framewrok shown before. We can specify a class (a collection) of pdfs that we will call $\mathcal{G}_p$:

- We seek within $\mathcal{G}$ the best approximation to the true model pdf $f(\boldsymbol{x}$, and we will call it $g(\boldsymbol{x}|\boldsymbol{\Theta})$.
- Such best approximation will minimize some calculated risk.

$$\mathrm{Loss}(f(\boldsymbol{x}), g(\boldsymbol{x}|\boldsymbol{\Theta}))) = \ln f(\boldsymbol{x}) - \ln g(\boldsymbol{x}|\boldsymbol{\Theta}))$$

with expected value, this is, the **risk** as

$$\ell(g) = \mathbb{E} \ln \frac{f(\boldsymbol{X})}{g(\boldsymbol{X}|\boldsymbol{\Theta})} = \int f(\boldsymbol{x}) \ln \frac{f(\boldsymbol{x})}{g(\boldsymbol{x}|\boldsymbol{\Theta})} \, \mathrm{d}\boldsymbol{x}$$

Train-Test-Validate

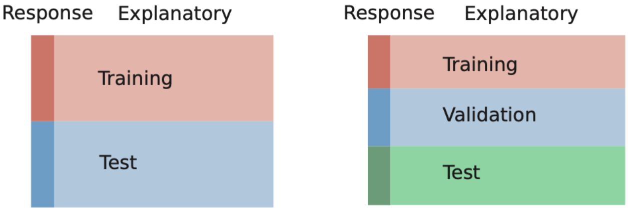


Figure 5: Sometimes we use the second set of data for model validation. Then we need to use a third one for testing.

Train-Test-Validate

To compare the predictive performance of various learners in $\mathcal{G}$, as measured by the test loss,

- we can use the same fixed training set τ and test set τ' for different learners, or
- if the overall data set is of modest size, we can perform the validation phase (model selection) on the training set only, using **cross-validation**.

Polynomial regression. Original data.

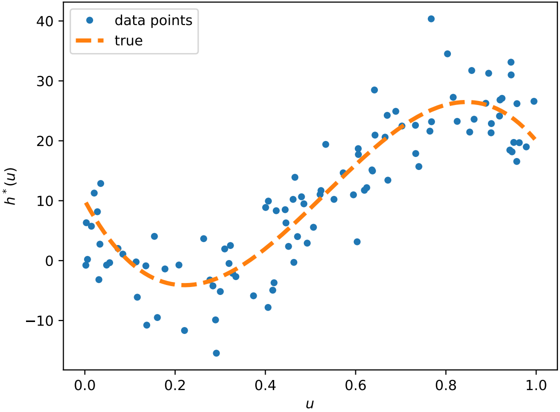


Figure 6: Training data and the optimal polynomial prediction function h^*[1]

Polynomial regression. Fitting.

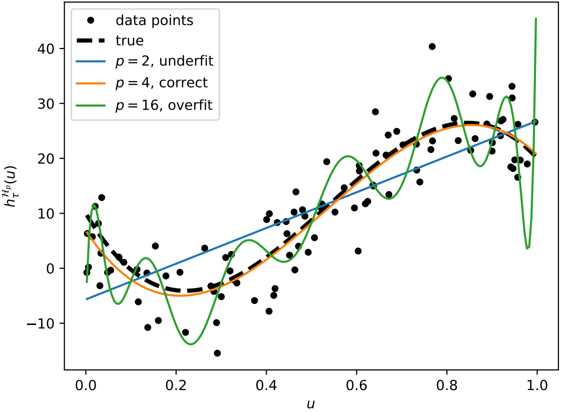


Figure 7: Fitted models for different orders of polynomial regressions[1].

Polynomial regression. Error.

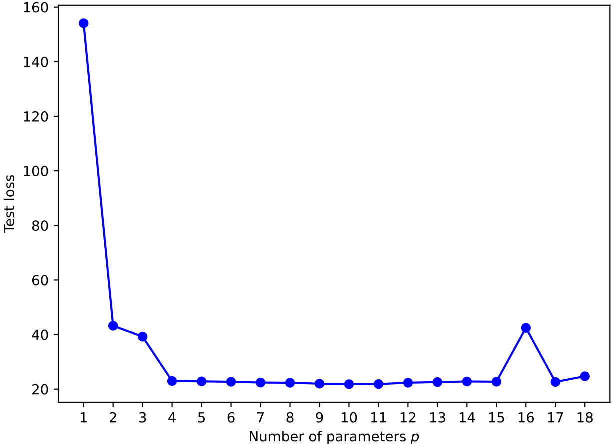


Figure 8: Fitted models for different orders of polynomial regressions[1].

Polynomial regression. Cross validation.

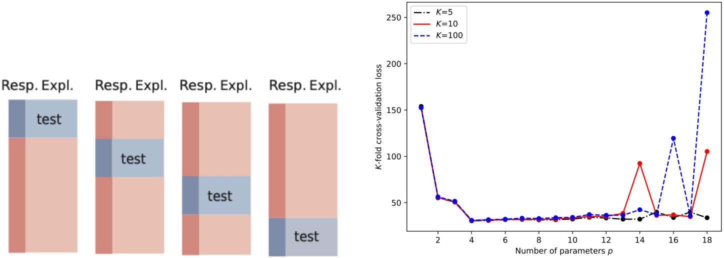


Figure 9: a) Example of four-fold cross-validation, representing four copies of the same data set. The data in each copy is partitioned into a training set (pink) and a test set (blue). Darker columns are the response variable; and lighter ones the explanatory variables. b) K-fold cross-validation for the polynomial regression[1].

- Dirk P. Kroese, Zdravko Botev, Thomas Taimre, and Radislav: Vaisman.
  Data Science and Machine Learning: Mathematical and Statistical Methods.
  Machine Learning & Pattern Recognition. Chapman & Hall/CRC, 2020.

- Junjie Peng, Elizabeth Jury, Pierre Dönnes, and Coziana Ciurtin.
  Machine Learning Techniques for Personalised Medicine Approaches in Immune-Mediated Chronic Inflammatory Diseases: Applications and Challenges.
  Frontiers in Pharmacology, 12, September 2021.

Annex: detailed notation I

Given an input or *feature* vector $\boldsymbol{x}$, ML aims at predicting an ouput or *response* variable vector $\boldsymbol{y}$. In particular, we search for a mathematical *prediction function* g such that we can *guess* an approximation to $\boldsymbol{y}$, $\hat{\boldsymbol{y}}$:

$$\begin{aligned} g \colon \mathcal{X} &\to \mathcal{Y} \\ \boldsymbol{x} &\mapsto \hat{\boldsymbol{y}} = g(\boldsymbol{x}) \end{aligned}$$

Definition

Dataset $S = \{\boldsymbol{z}_i\}_{i=1}^{n} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{n}$ is sampled from a distribution $\mathcal{D}$ over a domain $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$.
$\mathcal{X}$ is the instance domain (a set), $\mathcal{Y}$ is the label domain (a set), and $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ is the example domain (a set).

Annex: detailed notation II

Usually, $\mathcal{X}$ is a subset of $\mathbb{R}^d$ and $\mathcal{Y}$ is a subset of $\mathbb{R}^{d_o}$, where d is the input dimension, d_o is the output dimension.
$n = \#S$ is the number of samples. Without specification, S and n are for the training set.

- In *regression* problems, $\boldsymbol{y}$ is a vector of real values.
- In *classification* problems, $\boldsymbol{y}$ values lie within a finite set of c categories: $y \in \{0, 1, \ldots, c-1\}$.

Definition

A hypothesis space is denoted by $\mathcal{H}$. A hypothesis function is denoted by $f_{\boldsymbol{\theta}}(\boldsymbol{x}) \in \mathcal{H}$ or $f(\boldsymbol{x}; \boldsymbol{\theta}) \in \mathcal{H}$ with $f_{\boldsymbol{\theta}} : \mathcal{X} \to \mathcal{Y}$.

$\boldsymbol{\theta}$ denotes the set of parameters of $f_{\boldsymbol{\theta}}$.
If there exists a target function, it is denoted by f^*or $f : \mathcal{X} \to \mathcal{Y}$ satisfying $\boldsymbol{y}_i = f^*(\boldsymbol{x}_i)$ for $i = 1, \ldots, n$.

Annex: detailed notation III

A loss function, denoted by $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}_+ := [0, +\infty)$, measures the difference (or error) between a predicted label and a true label, e.g., L^2 loss:

$$\ell(f_{\boldsymbol{\theta}}, \boldsymbol{z}) = \frac{1}{2}(f_{\boldsymbol{\theta}}(\boldsymbol{x}) - \boldsymbol{y})^2,$$

where $\boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{y})$. $\ell(f_{\boldsymbol{\theta}}, \boldsymbol{z})$ can also be written as

$$\ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}), \boldsymbol{y})$$

for convenience.
(In the case of a classification, $\ell(f_{\boldsymbol{\theta}}, \boldsymbol{y}) = \mathbb{1}\{y \neq \hat{\boldsymbol{y}}\}$)
We will see other useful loss functions ({em cross entropy} or *hinge* loss functions) later in this course.
It is unlikely that a mathematical function $g \equiv \ f_{\boldsymbol{\theta}} : \mathcal{X} \to \mathcal{Y}$ would be able to make accurate predictions of all possible pairs $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$.

Annex: detailed notation IV

So, we use a probabilistic approach here to mpirical risk or training loss for a set $S = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{n}$ is denoted by $L_S(\boldsymbol{\theta})$ or $L_n(\boldsymbol{\theta})$ or $R_n(\boldsymbol{\theta})$ or $R_S(\boldsymbol{\theta})$,

$$L_S(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i). \tag{1}$$

The population risk or expected loss is denoted by $L_{\mathcal{D}}(\boldsymbol{\theta})$ or $R_{\mathcal{D}}(\boldsymbol{\theta})$

$$L_{\mathcal{D}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathcal{D}}\ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}), \boldsymbol{y}), \tag{2}$$

where $\boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{y})$ follows the distribution $\mathcal{D}$.
(In the case of a classification, we denote $L_{\mathcal{D}}(g) \equiv L_{\mathcal{D}}(\boldsymbol{\theta}) = \mathbb{P}_{\mathcal{D}}[f_{\boldsymbol{\theta}}(\boldsymbol{x}) \neq \boldsymbol{y}]$ and we say that g is a classifier.)
Because we are interested in minimizing the risk in our prediction, we are looking for the best possible $g^* := \operatorname{argmin}_g \mathbb{E}_{\mathcal{D}}\ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}), \boldsymbol{y})$

Annex: detailed notation V

(In classification, we look for $g^*(\boldsymbol{x}) = \underset{y \in \{0,1,\ldots,c-1\}}{\operatorname{argmax}} \mathbb{P}[Y = y \ X = x]$.)

Theorem

For the squared-error loss $\ell(y, \hat{y}) = (y - \hat{y})^2$, the optimal prediction function g^* is equal to the conditional expectation of Y given $\boldsymbol{X} = \boldsymbol{x}$.

which leads to write the random response Y as:

$$Y = g^*(\boldsymbol{x}) + \varepsilon(\boldsymbol{x})$$

Note that such random deviation satisfies $\mathbb{E}\varepsilon(\boldsymbol{x}) = 0$