

Statistical Learning

Chapter 1. Overview of Supervised learning

Pedro Delicado and Alex Sanchez

UPC & UB

Outline

- 1 Supervised and Unsupervised learning
- 2 Statistical Decision Theory
- 3 Regression Problems
- 4 Classification problems

Supervised Learning (the prediction problem)

- Let (X, Y) be a r.v. with support $\mathcal{X} \times \mathcal{Y} \subseteq \mathbb{R}^p \times \mathbb{R}$.
- General supervised learning or prediction problem:
 - Training sample: $S = \{(x_1, y_1), \dots, (x_n, y_n)\}$, i.i.d. from (X, Y) .
 - The goal is to define a function (possibly depending on the sample) $h_S : \mathcal{X} \mapsto \mathcal{Y}$ such that for a new independent observation (x_{n+1}, y_{n+1}) , from which we only know x_{n+1} , it happens that:

$$\hat{y}_{n+1} = h_S(x_{n+1}) \text{ is close to } y_{n+1} \text{ (in some sense).}$$

- Function h_S is called generically a *prediction function*. (or classification function or regression function, depending on the case).

Classification and Regression problems

The prediction function h_S is said to describe a *classification* or a *regression* problem depending on the case.

- If $\mathcal{Y} \subseteq \mathbb{R}$ (or \mathcal{Y} an interval) we have a standard *regression problem*.
 - Example: *Relating Salary and demographic variables*
- If $\mathcal{Y} = \{0, 1\}$ (or, also, $\mathcal{Y} = \{-1, 1\}$) we have a problem of *binary classification* or discrimination.
 - Example: *Predicting if a COVID patient will require (or not) ICU*
- If $\mathcal{Y} = \{1, \dots, K\}$ (or $\mathcal{Y} = \{y \in \{0, 1\}^K : \sum_{k=1}^K y_k = 1\}$) we face a of K classes classification problem.
 - Example: *Classifying a tumor into one of many types*

Supervised learning

- Probabilistic model for supervised learning
 - Response variable Y .
 - Explanatory variables (features) $X = (X_1, \dots, X_p)$.
 - Data $(x_i = (x_{i1}, \dots, x_{ip}), y_i), i = 1, \dots, n$ i.i.d. from the random variable

$$(X = (X_1, \dots, X_p), Y) \sim \Pr(X, Y)$$

- $\Pr(X, Y)$ denotes the joint distribution of X and Y .
 - When this joint distribution is continuous, $\Pr(X, Y)$ is the joint probability density function.

- Main interest is *predicting* Y from X .
- Given the probabilistic model it can be re-stated as *learning the conditional distribution* $\Pr(Y \mid X)$.
- In practice we focus on *learning a conditional location parameter*:

$$\mu(x) = \operatorname{argmin}_{\mu} \mathbb{E}(L(Y, \mu) \mid X = x),$$

where $L(y, \hat{y})$, loss function, measures the error of predicting y with \hat{y} .

- For quadratic loss, $L(y, \hat{y}) = (y - \hat{y})^2$, $\mu(x)$ is the regression function:

$$\mu(x) = \mathbb{E}(Y \mid X = x)$$

Unsupervised learning

- It aims at learning relationships and structure from the observed data.
- Probabilistic model:
 - Variables of interest: $X = (X_1, \dots, X_p)$.
 - Data $x_i = (x_{i1}, \dots, x_{ip})$, $i = 1, \dots, n$ i.i.d. from the random variable

$$X = (X_1, \dots, X_p) \sim \Pr(X).$$

- $\Pr(X)$ denotes the probability distribution of X .
 - If X is continuous, $\Pr(X)$ is the probability density function of X .
- Main interest: To infer properties of $\Pr(X)$.

Specific problems in unsupervised learning:

- Estimating directly the density function $\Pr(x)$:
 - Density estimation (histogram, kernel densities, Gaussian MM)
- Detecting homogeneous subpopulations C_1, \dots, C_k s.t.:

$$\Pr(x) = \sum_{j=1}^k \alpha_j \Pr(x | C_j), \alpha_j \geq 0, \sum_j \alpha_j = 1.$$
 - Clustering (hierarchical clustering, k -means, ...)
- Finding low-dimensional hyper-planes or hyper-surfaces (manifolds) in \mathbb{R}^p around which the probability $\Pr(x)$ is concentrated.
 - Dimensionality reduction (PCA, MDS, Manifold learning ...)
- Proposing generative probabilistic models for X , depending on low-dimensional unobservable random variables F .
 - Extraction of latent variables (Factor Analysis, ...)

Statistical Decision Theory

- The *prediction problem* can be written as a *decision problem* which can be casted in the setting of *Statistical Decision Theory*.
- Let (X, Y) be a r.v. with support $\mathcal{X} \times \mathcal{Y} \subseteq \mathbb{R}^p \times \mathbb{R}$.
- Prediction problem: To look for a prediction function $h : \mathcal{X} \mapsto \mathcal{Y}$ such that $h(X)$ is close to Y in some sense.
- The (lack of) closeness between $h(X)$ and Y is usually measured by a loss function $L(Y, h(X))$.
 - For instance, the squared error loss is $L(Y, h(X)) = (Y - h(X))^2$.
 - $L(Y, h(X))$ is a r.v., with expected value $\text{EL}(h) = \mathbb{E}(L(Y, h(X)))$, called expected loss, that only depends on h .
- Decision problem: To find the prediction function $h : \mathcal{X} \mapsto \mathcal{Y}$ that minimizes the expected loss.

Bayes rule

- Denote by $\Pr_{(X,Y)}(x,y)$ the joint probability distribution of (X,Y) .
- Observe that, for any $h : \mathcal{X} \mapsto \mathcal{Y}$ a lower bound for $\text{EL}(h)$ can be set as follows:

$$\begin{aligned}\text{EL}(h) &= \mathbb{E}(L(Y, h(X))) \\ &= \int_{\mathcal{X} \times \mathcal{Y}} L(y, h(x)) d\Pr_{(X,Y)}(x, y) \\ &= \int_{\mathcal{X}} \left(\int_{\mathcal{Y}} L(y, h(x)) d\Pr_{Y|X=x}(y) \right) d\Pr_X(x) \\ &= \int_{\mathcal{X}} \mathbb{E}(L(Y, h(x)) \mid X = x) d\Pr_X(x) \\ &\geq \int_{\mathcal{X}} \min_{y \in \mathcal{Y}} \mathbb{E}(L(Y, y) \mid X = x) d\Pr_X(x) \\ &= \text{EL}(h_B) .\end{aligned}$$

- From the previous bound: $EL(h) \geq EL(h_B)$, it follows that, given a loss function $L(y, h(x))$ no prediction function can be better than the Bayes rule, or equivalently, that
- The optimal prediction function is the Bayes rule or Bayes classifier defined as:

$$h_B(x) = \arg \min_{y \in \mathcal{Y}} \mathbb{E}(L(Y, y) \mid X = x).$$

The regression problem

- Let (X, Y) be a $(p + 1)$ -dimensional random variable, with $Y \in \mathbb{R}$.
- The regression problem: To predict Y from known values of X .
- The most common (and convenient) approach is to adopt as loss function is the *squared error loss*:
$$L(Y, h(X)) = (Y - h(X))^2 .$$
- Expected loss known as *Prediction Mean Squared Error*, (*PMSE*):

$$\text{PMSE}(h) = \mathbb{E} ((Y - h(X))^2) .$$

- The Bayes rule in this case is

$$h_B(x) = \arg \min_{y \in \mathcal{Y}} \mathbb{E} ((Y - y)^2 \mid X = x) .$$

- Observe that, for any $y \in \mathcal{Y}$ one can decompose the conditional expectation of the squared deviation between Y and y given $X = x$, $\mathbb{E}((Y - y)^2 | X = x)$ in such a way that:

$$\begin{aligned}\mathbb{E}((Y - y)^2 | X = x) &= \\&= \mathbb{E}(((Y - \mathbb{E}(Y | X = x)) + (\mathbb{E}(Y | X = x) - y))^2 | X = x) \\&= \mathbb{E}((Y - \mathbb{E}(Y | X = x))^2 | X = x) + \underbrace{(\mathbb{E}(Y | X = x) - y)^2}_{\geq 0} \\&\quad + 2(\mathbb{E}(Y | X = x) - y)\mathbb{E}(Y - \mathbb{E}(Y | X = x) | X = x) \\&\geq \mathbb{E}\left((Y - \underbrace{\mathbb{E}(Y | X = x)}_{h_B(x)})^2 | X = x\right)\end{aligned}$$

Optimal predictor in regression

- From the previous development it yields that, for regression problems, the Bayes rule is the conditional expectation of Y given $X = x$,

$$h_B(x) = \mathbb{E}(Y \mid X = x),$$

- It is also known as regression function of Y over x and is usually denoted by

$$m(x) = \mathbb{E}(Y \mid X = x).$$

Parametric regression

- Parametric regression models assume that $m(x)$ is known except for a finite number of unknown parameters,

$$m(x) \equiv m(x; \theta), \theta \in \Theta \subseteq \mathbb{R}^q,$$

- For instance, the multiple linear regression model postulates that $m(x) = \beta_0 + x^\top \beta_1$, with unknown parameters $\beta_0 \in \mathbb{R}, \beta_1 \in \mathbb{R}^p$.
- A training sample, $S = \{(x_1, y_1), \dots, (x_n, y_n)\}$, i.i.d. from (X, Y) , is used to estimate the parameter θ .
- In this case $h_S(x) = m(x; \hat{\theta})$, where $\hat{\theta} = \hat{\theta}(S)$ is the estimation of θ from sample S .

Least squares estimation

- A usual way to estimate θ in parametric models is by least squares:

$$\hat{\theta} = \arg \min_{\theta \in \Theta} \sum_{i=1}^n (y_i - m(x_i; \theta))^2$$

- The regression function $m(x)$ is linear in x .
- It can be shown that, independently of the distributions, $\hat{\theta}$ is the Best Linear Unbiased Estimator (BLUE) of θ .
- Assuming joint normality for X and Y the LS-estimator is equivalent to the maximum likelihood estimator of θ
- In this case, the model is $Y = m(X) + \varepsilon$, where ε is an additive noise normally distributed with zero mean and independent from X , also normally distributed.

Least squares estimation and prediction errors

- The LS estimator $\hat{\theta}$ minimizes the prediction error, RSS, in the training sample.
- That is, the Residual Sum of Squares,

$$\text{RSS}(\theta) = \sum_{i=1}^n (y_i - m(x_i; \theta))^2,$$

takes its minimum value when $\theta = \hat{\theta}$

$$\overline{\text{err}} = \text{RSS}(\hat{\theta}) = \sum_{i=1}^n (y_i - m(x_i; \hat{\theta}))^2$$

Different types of prediction error

- $\text{RSS}(\theta)$ is the *prediction error* a theoretical quantity, based on the training sample, that needs to be estimated.
- $\overline{\text{err}}$, known as the *training error* or the *apparent error*, is an approximation to $\text{RSS}(\theta)$.
- We are interested in the error associated when predicting a new observation, that is the Prediction Mean Squared Error (PMSE)

$$\text{PMSE}(\theta) = \mathbb{E} \left((Y_{n+1} - m(x_i; \theta))^2 \right),$$

- $\overline{\text{err}}$ is an optimistic estimation of the in an observation of (X_{n+1}, Y_{n+1}) independent from the training sample,

$\overline{\text{err}}$ and PMSE are not the same

- In some cases such as in linear regression $\overline{\text{err}}$ is a good approximation to $\min_{\theta \in \mathbb{R}^q} \text{PMSE}(\theta)$
- But, when the parametric family $m(x; \theta), \theta \in \Theta \subseteq \mathbb{R}^q$, is too flexible:

$$\overline{\text{err}} < \text{PMSE}(\hat{\theta}) \neq \min_{\theta \in \mathbb{R}^q} \text{PMSE}(\theta)$$

- This is the case in non-parametric regression and in many machine learning algorithms. (Example: k -nearest neighbors regression, where the tuning parameter is k).
- We will talk later in the course about cross-validation and tuning parameters.

k nearest-neighbors regression

- K-NN is a flexible approach to regression or classification that, instead of relying on a *global model* based on all observations models each observation locally based on its *nearest neighbors*.
- The k nearest-neighbor estimator of $m(t) = E(Y \mid X = t)$ is:

$$\hat{m}(t) = \frac{1}{|N_k(t)|} \sum_{i \in N_k(t)} y_i,$$

where $N_k(t)$ is the neighborhood of t defined by the k closest points x_i in the training sample.

- Closeness is defined according to a previously chosen distance measure $d(t, x)$, for instance, the Euclidean distance.

K-NN is flexible or way too flexible

- K-NN regression is a great real-world example of how model flexibility impacts training error vs. prediction error:
 - When $k=1$ the model memorizes training data, leading to zero training error.
 - However, for a new test observation, predictions are **highly unstable** (high variance): $\text{PMSE}(\hat{\theta}) \gg \overline{\text{err}}$.
 - As k increases, the model becomes less flexible, reducing variance but increasing bias.
 - The optimal k balances both, minimizing PMSE
- **Conclusion:** Overly flexible models, like small k in k -NN, cause **training error to be misleading**.

Practice session

- The R notebook `knn_regr.Rmd` illustrates the advantages and drawbacks of K-NN regression using R.
- Run along it and experiment with different settings.

The classification problem

- Let (X, Y) be a r.v. with support $\mathcal{X} \times \mathcal{Y} \subseteq \mathbb{R}^p \times \{1, \dots, K\}$.
- We want to predict Y from observed values of X .
- The loss function in this case can be represented by a $K \times K$ matrix L , that will be zero on the diagonal and nonnegative elsewhere.
 - The element (j, k) of L is $L(j, k)$: the price paid for classifying in class k an observation belonging to class j .

The zero-one loss function

- A common loss function for classification is the zero-one loss function is used, where *all misclassifications are charged a single unit*.
- With the 0-1 loss function the Bayes rule is

$$\begin{aligned}h_B(x) &= \arg \min_{y \in \mathcal{Y}} \mathbb{E} (L_{0-1}(Y, y) \mid X = x) \\&= \arg \min_{k \in \{1, \dots, K\}} \sum_{j=1}^K L_{0-1}(j, k) \Pr(Y = j \mid X = x) \\&= \arg \min_{k \in \{1, \dots, K\}} (1 - \Pr(Y = k \mid X = x)) \\&= \arg \max_{k \in \{1, \dots, K\}} \Pr(Y = k \mid X = x).\end{aligned}$$

- In this context the Bayes rule is known as the Bayes classifier, and says that we classify to the most probable class, conditional to the observed value x of X .

The problem of binary classification

- In the binary classification problem: $\mathcal{Y} = \{0, 1\}$. Then $(Y \mid X = x) \sim \text{Bernoulli}(p = p(x) = \Pr(Y = 1 \mid X = x) = \mathbb{E}(Y \mid X = x))$.

- The Bayes classifier is

$$h_B(x) = \begin{cases} 1 & \text{if } p(x) \geq 1/2 \\ 0 & \text{if } p(x) < 1/2 \end{cases}$$

- As $p(x)$ is unknown, we use a training sample to estimate it.
- Let $(x_1, y_1), \dots, (x_n, y_n)$ be n independent realizations of (X, Y) .
- Given an estimation $\hat{p}(x)$ of the regression function $p(x)$, the estimated version of the Bayes classifier is

$$h_S(x_{n+1}) = \begin{cases} 1 & \text{if } \hat{p}(x_{n+1}) \geq 1/2 \\ 0 & \text{if } \hat{p}(x_{n+1}) < 1/2 \end{cases}$$

Parametric estimation in binary classification

- In parametric modeling it is assumed that $p(x) = \Pr(Y = 1 \mid X = x)$ is known except for a finite number of unknown parameters,

$$p(x) \equiv p(x; \theta), \theta \in \Theta \subseteq \mathbb{R}^q.$$

- The likelihood and log-likelihood are, respectively:

$$L(\theta) = \prod_{i=1}^n \Pr(Y_i = y_i \mid X_i = x_i) = \prod_{i=1}^n p(x_i; \theta)^{y_i} (1 - p(x_i; \theta))^{1-y_i}$$

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^n (y_i \log p(x_i; \theta) + (1 - y_i) \log (1 - p(x_i; \theta)))$$

- Let $\hat{\theta} = \arg \max_{\theta \in \Theta} \ell(\theta)$ be the maximum likelihood estimator of θ .
- Then $\hat{p}(x) = p(x; \hat{\theta})$ is used to define the classification rule.

Other optimization criteria for binary classification

- Maximum likelihood is not the only possibility for estimating θ in $p(x; \theta)$.
- Alternatives:
 - Minimization of the misclassification error:

$$\hat{\theta}_{\text{Miss}} = \arg \min_{\theta \in \Theta} \sum_{i=1}^n (y_i - \mathbb{I} \{p(x_i; \theta) \geq 0.5\})^2.$$

- Least squares estimation:
$$\hat{\theta}_{LS} = \arg \min_{\theta \in \Theta} \sum_{i=1}^n (y_i - p(x_i; \theta))^2.$$
- Least absolute deviation:
$$\hat{\theta}_{LAD} = \arg \min_{\theta \in \Theta} \sum_{i=1}^n |y_i - p(x_i; \theta)|.$$
- Penalized version of these criteria, when the statistical model $p(x; \theta)$, $\theta \in \mathbb{R}^q$, is too flexible.

k-Nearest Neighbors (k-NN) for classification

k-Nearest Neighbors (k-NN) is a simple and effective classification method.

It relies on the idea that similar instances should belong to the same class.

- Given a training set (\mathcal{T}) with labeled instances (x_i, y_i) ,
- To classify a new instance x , we:
 - 1 Find the k closest points x_i to x .
 - 2 Take the *majority vote\$ of their corresponding labels y_i .

The decision boundary of k-NN is **nonlinear** and **flexible**, adapting to local patterns in the data.

k-NN Classification Model

The prediction for a new point (x) is given by:

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

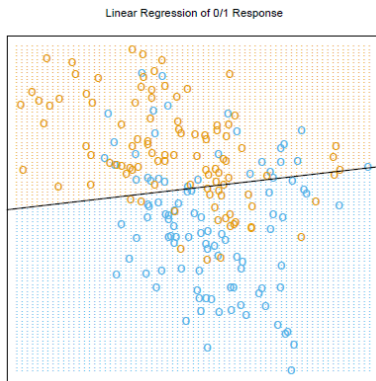
where:

- $N_k(x)$ is the set of the k nearest neighbors of x .
- y_i are the corresponding labels (0 or 1 in binary classification).
- Closeness is typically measured using **Euclidean distance**.

For classification:

- If $\hat{Y}(x) > 0.5$, classify as **Class 1**.
- Otherwise, classify as **Class 0**.

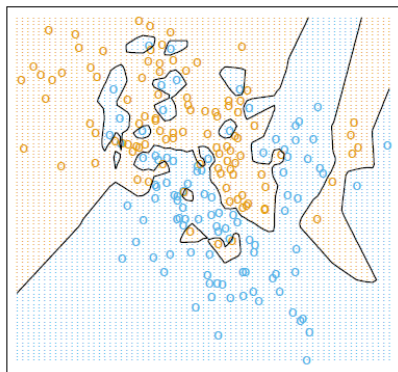
Decision Boundaries - Linear Regression vs. k-NN



- Linear regression fits a straight line decision boundary: ($x^T \hat{\beta} = 0.5$).
- Misclassifications occur because it assumes a **linear separation**.
- It does not capture **local structures** in the data.

- ◀ ◻ ▶ ◀ ◻ ▶ ◀ ≡ ▶ ◀ ≡ ▶ ≡ 🔍 ↺

k-NN with $k=1$



- 1-NN assigns the label of the **single closest** training point.
- Each point belongs to the nearest neighbor's class: **Voronoi tessellation**.
- Decision boundary is **highly irregular** and sensitive to noise.

Choosing k in k -NN

- The parameter k in K -NN reflects its flexibility
 - $k=1$ leads to **overfitting**, that is, perfect accuracy on training but poor generalization.
 - Larger k smooths the decision boundary but might **lose fine details**.
- **Trade-offs:**
 - Small (k) : **low bias, high variance**.
 - Large (k) : **high bias, low variance**.
 - **Optimal k** is chosen via cross-validation (later in the course) that aims at balancing the former error measures.

Summary

- k-NN is **flexible** and works well for complex decision boundaries.
- It is **non-parametric** and **data-driven**.
- The choice of (k) is critical for **generalization**.
- Compared to linear regression, k-NN adapts better to **nonlinear class distributions**.

k -nn classification, in R

Follow the Rmd files

`SimMixtNorm.Rmd` and `knn_class.Rmd`

Evaluating a binary classification rule

- The explanation has been removed
- Instead you can follow the slides of a talk on Biomarkers where classification performance for binary classifiers is discussed
 - [Link to the slides](#)

Main references