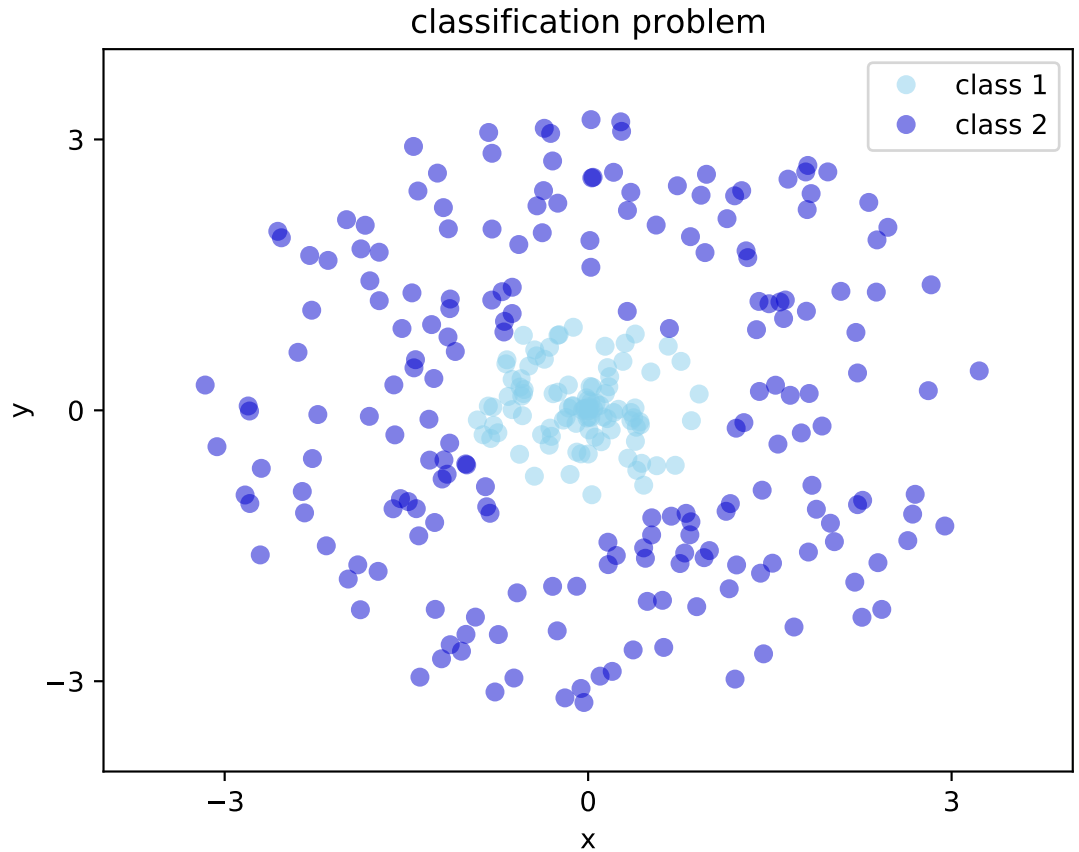
Fondamentaux théoriques du machine learning



Overview of lecture 4

Ridge regression

- Summary of OLS
- Ridge regression estimator
- Cross validation
- Numerical resolution of OLS and Ridge regression

Feature maps

Classification

- Problem statement
- Convexification of the risk and calibration
- Logistic regression
- Maximum likelihood

Why study OLS

- Illustrates the bias-variance decomposition
- Can be extended to non-linear features (see section II)

Summary

- If X is injective, then we have a closed form solution :

$$\hat{\theta} = (X^T X)^{-1} X^T y \tag{1}$$

- Risk decomposition

$$E[R_X(\theta)] - R_X(\theta^*) = ||E[\theta] - \theta^*||^2_{\hat{\Sigma}} + E\left[||\theta - E[\theta]||^2_{\hat{\Sigma}}\right]$$

- Ecess risk :

$$E[R_X(\hat{\theta})] - R_X(\theta^*) = \frac{\sigma^2 d}{n} \tag{2}$$

Expected value of empirical risk

Proposition

The expected value of the empirical risk of $\hat{\theta}$ writes :

$$E[R_n(\hat{\theta})] = \frac{n-d}{n}\sigma^2 \tag{3}$$

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Exercice 1 : **Variance estimation.** Could we use this to estimate the variance ?

Expected value of empirical risk

Proposition

$$E[R_n(\hat{\theta})] = \frac{n-d}{n}\sigma^2 \tag{5}$$

Two consequences :

- In expectation, the amount of overfitting is $\frac{2\sigma^2}{n}$.
- We can have an **unbiased estimator** of the variance σ^2 with :

$$\frac{||Y - X\hat{\theta}||_2^2}{n-d} \tag{6}$$

Issues in high dimension

The problem can become **ill-conditioned**.
When d is large (for instance when $\frac{d}{n}$ is close to 1), then

- the amount of excess risk is not way smaller than σ^2.
- if $d = n$ and $X^T X$ is invertible, we can fit the training data exactly, which is bad for generalization.

If $d > n$, $X^T X$ is not invertible, we do not have a closed form solution anymore, we can have a subspace of solutions.
Remark : in low d as well, the problem can be ill-conditioned (for instnace is X has colinear columns).

Regularization

To avoid these problems, a solution is to perform **regularization** of the objective function.
Regularizing the problem is an approach to enforce the unicity of the solution at the cost of introducing a **bias** in the estimator. The unicity is garanteed by the **strong convexity** of the new loss function.

Ridge regression estimator

$$\hat{\theta}_\lambda = \underset{\theta \in \mathbb{R}^d}{\arg\min} \left(\frac{1}{n} ||Y - X\theta||_2^2 + \lambda ||\theta||_2^2 \right) \tag{7}$$

with $\lambda > 0$.

RIdge regression estimator

Proposition

The Ridge regression estimator is unique even if $X^T X$ is not inversible and is given by

$$\hat{\theta}_\lambda = \frac{1}{n}(\hat{\Sigma} + \lambda I_d)^{-1} X^T Y$$

with

$$\hat{\Sigma} = \frac{1}{n} X^T X \in \mathbb{R}^{d,d} \tag{8}$$

Proof

Step 1 : Prove that the loss $R_n(\theta)$ 7 is strongly convex.

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- $x \mapsto ||\theta||^2$ is 2-convex on $\mathbb{R}^d$
  - $\theta \mapsto \theta_i$ is linear
  - $u \mapsto u^2$ is 2-convex on $\mathbb{R}$
- $R_n(\theta)$ is a sum of a convex function and $\theta \mapsto \lambda||\theta||_2^2$.

Proof

Step 2 : as $R_n(\theta)$ is strongly convex, there exists a unique minimizer obtained by cancellation of the gradient.
Compute the gradient of $R_n(\theta)$.

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Compute the gradient of $R_n(\theta)$.

$$\nabla_\theta R_n(\theta) = \frac{2}{n}(X^T X\theta - X^T y) + 2\lambda\theta$$

Proof

The equation of the cancellation of the gradient is

$$(\frac{2}{n}n\hat{\Sigma} + 2\lambda I_d)\theta_\lambda = \frac{2}{n}X^T y$$

which we can write

$$n(\hat{\Sigma} + \lambda I_d)\theta_\lambda = X^t y$$

Proof

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which we can write

$$n(\hat{\Sigma} + \lambda I_d)\theta_\lambda = X^t y$$

$\hat{\Sigma} + 2\lambda I_d$ is a symmetric matrix with all eigenvalues $\geq 2\lambda$. Thus, it is invertible. Also, $\forall a \in \mathbb{R}^*$ and $A \in GL_d\mathbb{R}$, $(aA)^{-1} = \frac{1}{a}A^{-1}$, which concludes the proof.

Statistical analysis of ridge regression

Proposition

Under the linear model assumption, with fixed design setting, the ridge regression estimator has the following excess risk

$$E[R(\hat{\theta}_\lambda] - R^* = \lambda^2 \theta^{*T} (\hat{\Sigma} + \lambda I_d)^{-2} \hat{\Sigma} \theta^* + \frac{\sigma^2}{n} tr[\hat{\Sigma}^2 (\hat{\Sigma} + \lambda I_d)^{-2}] \quad (9)$$

Choice of λ

Is it possible that the excess risk is smaller with risge regression than OLS ?

Proposition

With the choice

$$\lambda^* = \frac{\sigma\sqrt{tr(\hat{\Sigma})}}{||\theta^*||_2\sqrt{n}} \tag{10}$$

then

$$E[R(\hat{\theta}_\lambda] - R^* \leq \frac{\sigma\sqrt{tr(\hat{\Sigma})}||\theta^*||_2}{\sqrt{n}} \tag{11}$$

Choice of λ

$$E[R(\hat{\theta}_\lambda] - R^* \leq \frac{\sigma\sqrt{tr(\hat{\Sigma})}||\theta^*||_2}{\sqrt{n}} \tag{12}$$

- dimension-free bound
- $\frac{1}{n}$ (OLS) vs $\frac{1}{\sqrt{n}}$ (ridge), with different constants, dimension-free in ridge.

Hyperparameter

- In practical situations, the quantities involved in the computation of λ^* in 10 are typically unknown. However this equation show that there may exist a λ with a good prediction performance, which can be found by cross validation in practice.
- λ is an example of **hyperparameter**.

Hyperparameter

scikit

- cross validation
- grid search

Neural networks

With neural networks, it seems that it is possible to have $d >> n$ but no overfitting (simplicity bias). Why ?

Numerical resolution

- closed-form OLS and ridge estimator require matrix inversions.
- $\mathcal{O}(d^3)$ operation. This is prohibitive in large dimensions (e.g. $\geq 10^5$).
- **iterative algorithms** are preferred :
  - Gradient descent (GD)
  - Stochastic gradient descent (SGD)

Gradient descent

$$\theta \leftarrow \theta - \gamma \nabla_\theta f \tag{13}$$

γ is a parameter called the learning rate.

- We will study gradient algorithms later in the course
- In many cases, it is possible to compute explicit convergence rates.

Feature maps

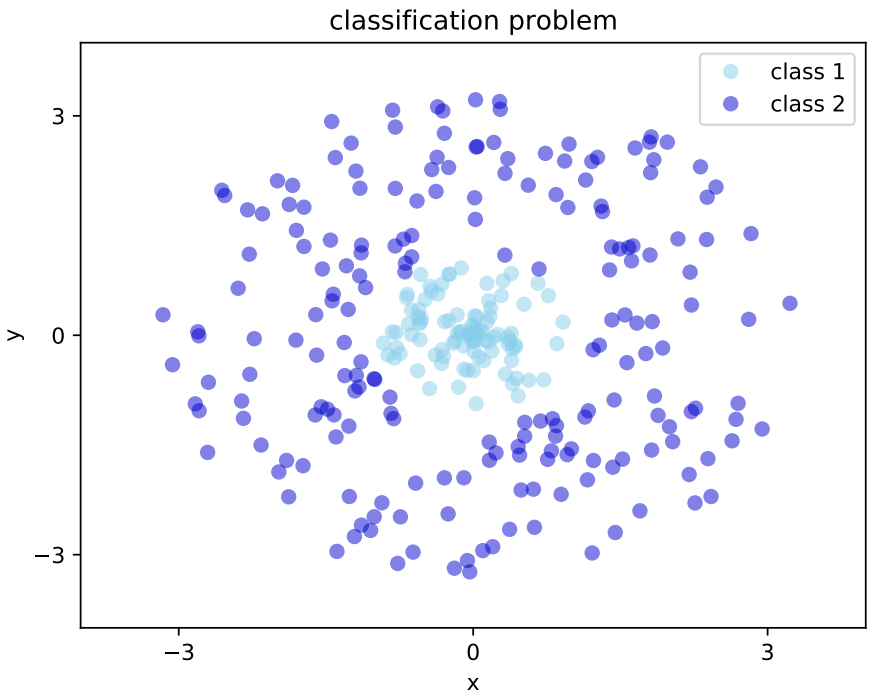
Often, we do not work with the $x_i \in \mathcal{X}$, but with **representations** $\phi(x_i)$, with $\phi : \mathcal{X} \to \mathbb{R}^d$. Possible motivations :

- $\mathcal{X}$ need not be a vector space.
- $\phi(x)$ can provide more useful **features** for the considered problem (classification, regression).
- The prediction function is then allowed to depend **non-linearly** on x.

Feature map

Exercice 2 : **Finding a feature map**

What feature map could be used to be able to linearly separate these data ?



Application to OLS and ridge

Instead of

$$X = \begin{pmatrix} x_1^T \\ \dots \\ x_i^T \\ \dots \\ x_n^T \end{pmatrix} = \begin{pmatrix} x_{11}, \dots, x_{1j}, \dots x_{1d} \\ \dots \\ x_{i1}, \dots, x_{ij}, \dots x_{id} \\ \dots \\ x_{n1}, \dots, x_{nj}, \dots x_{nd} \end{pmatrix}$$

The design matrix is

$$\phi = \begin{pmatrix} \phi(x_1)^T \\ \dots \\ \phi(x_i)^T \\ \dots \\ \phi(x_n)^T \end{pmatrix}$$

Application to OLS and ridge

The statistical results are maintained, as a function of d, the dimension of $\phi(x)$.

Linear estimator

We often encounter estimators of the form

$$f(x) = h(\langle \phi(x), \theta \rangle) = h(\phi(x)^T \theta) \tag{14}$$

- They are often called "linear models"
- Being linear in θ is not the same as being linear in x.

Linear estimator

We often encounter estimators of the form

$$f(x) = h(\langle \phi(x), \theta \rangle) = h(\phi(x)^T \theta) \tag{15}$$

- regression : $h = Id$
- classification : $h = \text{sign}$.

Linear estimator

Interpretation of a linear model as a vote, in the case of classification.

$$f(x) = h(\langle \phi(x), \theta \rangle) = h(\phi(x)^T \theta) \tag{16}$$

Kernel methods

The topic of feature maps is very rich and important in machine learning

- **kernel methods** : ϕ is **chosen**. Many famous choices are available (gaussian kernels, polynomial kernels, etc).
- **neural networks** : ϕ is **learned**.

We will have a dedicated course on both these methods.

General classification problem

- $\mathcal{X} = \mathbb{R}^d$
- $\mathcal{Y} = \{-1, 1\}$ or $\mathcal{Y} = \{0, 1\}$.
- $l(y, z) = 1_{y \neq z}$ ("0-1" loss)
- $F = \mathcal{Y}^{\mathcal{X}}$

Problem

Optimizing on $F = \mathcal{Y}^{\mathcal{X}}$ is equivalent to optimizing in the set of subsets of $\mathcal{X}$.
We cannot differentiate on this hypothesis space and it is not clear how to regularize.

Subsets

Exercice 3 : **Combinatorial problem**

If we wanted to try all applications in $\mathcal{Y}^{\mathcal{X}}$, if $|\mathcal{X}| = n$, how many applications would there be ?

Bayes predictor

Proposition

Law of total expectation

$$E_{X,Y}\Big[I(X,Y)\Big] = E_X\Big[E\big(I(X,Y)|X\big)\Big] \tag{17}$$

Bayes predictor

Hence,

$$f^*(x) = \arg\min_{z \in \mathcal{Y}} E\Big[I(y, z) | X = x \Big] \tag{18}$$

Bayes predictor

Reminder : if we assume the knowledge of the joint distribution (X, Y), the Bayes predictor can be explicitely computed.

$$\begin{aligned} f^*(x) &= \arg\min_{z \in \mathcal{Y}} E\Big[l(y,z)|X=x\Big] \\ &= \arg\min_{z \in \mathcal{Y}} P(Y \neq z|X=x) \\ &= \arg\min_{z \in \mathcal{Y}} 1 - P(Y=z|X=x) \\ &= \arg\max_{z \in \mathcal{Y}} P(Y=z|X=x) \end{aligned} \tag{19}$$

The optimal classifier selects the most probable output given $X = x$.

Bayes risk

$$
\begin{aligned}
R^* &= E\Big[I(Y, f^*(X))\Big] \\
&= E\Big[P(Y \neq f^*(X))\Big] \\
&= E_X\Big[E_Y\Big(P(Y \neq f^*(X)|X\Big)\Big] \\
&= E_X\Big[P(Y \neq f^*(X)|X)\Big]
\end{aligned}
\tag{20}
$$

Bayes risk

$$\begin{aligned} R^* &= E\Big[I(Y, f^*(X))\Big] \\ &= E\Big[P(Y \neq f^*(X))\Big] \\ &= E_X\Big[E_Y\Big(P(Y \neq f^*(X)|X\Big)\Big] \\ &= E_X\Big[P(Y \neq f^*(X)|X)\Big] \end{aligned} \tag{21}$$

But we have

$$P\big(Y \neq f^*(X)|X = x\big) = P\big(Y \neq f^*(x)\big) \tag{22}$$

Bayes risk

We note $\eta(x) = P(Y = 1|X = x)$. Then,

- If $\eta(x) > \frac{1}{2}$, then $f^*(x) = 1$, and $P\big(Y \neq f^*(x)\big) = P\big(Y = 0\big) = 1 - \eta(x)$
- If $\eta(x) < \frac{1}{2}$, then $f^*(x) = 0$, and $P\big(Y \neq f^*(x)\big) = P\big(Y = 1\big) = \eta(x)$

In both cases, $P\big(Y \neq f^*(x)\big) = \min(\eta(x), 1 - \eta(x))$.
We conclude that

$$R^* = E_X\Big[\min(\eta(X), 1 - \eta(X))\Big] \tag{23}$$

Exercice 4 : Same random variable (X, Y) as in lecture 3, with $p = 1/3$, $q = 3/4$.

- $\mathcal{X} = \{0, 1\}$, $\mathcal{Y} = \{0, 1\}$.
- $X \sim B(\frac{1}{2})$,

$$Y = \begin{cases} B(1/3) \text{ if } X = 1 \\ B(3/4) \text{ if } X = 0 \end{cases}$$

With $B(p)$ a Bernoulli law with parameter p.

Compute the Bayes estimator and the bayes risk.

Bayes estimator

Bayes estimator

- $f^*(0) = 1$
- $f^*(1) = 0$
- $\eta(1) = \frac{1}{3}$
- $\eta(0) = \frac{3}{4}$

$$R^* = \frac{7}{24} \tag{24}$$

Real-valued function

Instead of an application in $\mathcal{Y}^{\mathcal{X}}$, we will learn $g : \mathcal{X} \to \mathbb{R}$ and define $f(x) = \text{sign}(g(x))$ with

$$\text{sign}(x) = \begin{cases} 1 \text{ if } x \geq 0 \\ -1 \text{ if } x < 0 \end{cases}$$

Risk

The risk (generalization error) of $f = \text{sign} \circ g$ is defined as

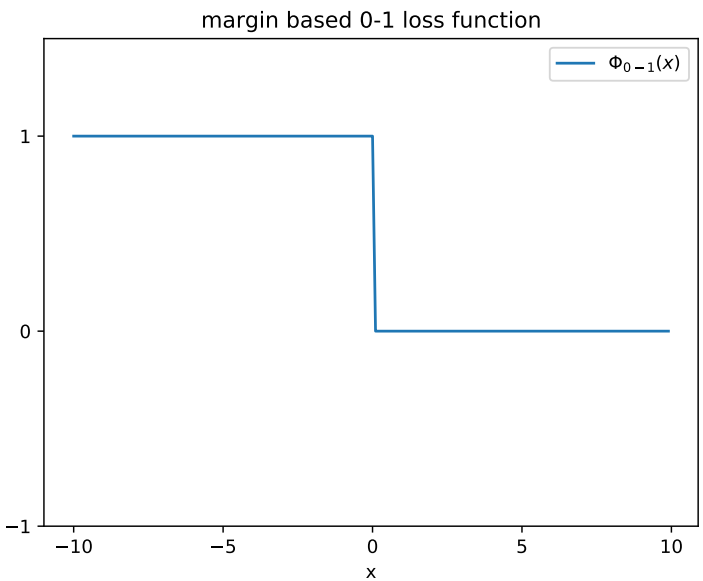
$$\begin{aligned} R(g) &= P(\text{sign}(g(x)) \neq y) \\ &= E\left[1_{\text{sign}(g(x)) \neq y}\right] \\ &= E\left[1_{yg(x)<0}\right] \end{aligned} \tag{25}$$

Several solutions

There might be many optimal functions g, i.e : such that $\text{sign}(g(x)) = f^*(x)$.

Margin based 0-1 loss function Φ_{0-1}

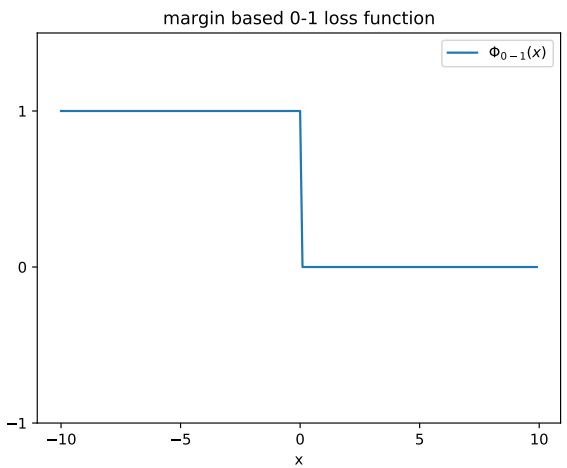
$$\begin{aligned} R(g) &= E\left[1_{\text{sign}(g(x))\neq y}\right] \\ &= E\left[1_{yg(x)<0}\right] \\ &= E\left[\Phi_{0-1}(yg(x))\right] \end{aligned} \tag{26}$$



Empirical risk minimization

The corresponding empirical risk writes :

$$\frac{1}{n}\sum_{i=1}^{n}\Phi_{0-1}(y_i g(x_i)) \tag{27}$$



What is the issue with this objective function ?

Empirical risk minimization

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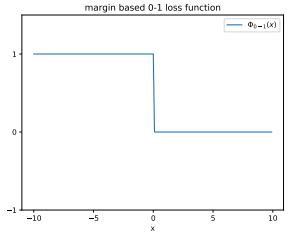

What is the issue with this objective function ?

- non-convex
- not continuous

Convex surrogate

Key idea : replace Φ_{0-1} by another function Φ that is easier to optimize (convexity) but still represents the correctness of the classification.

Definition

The Φ-risk is defined as

$$R_\Phi(g) = E\Big[\Phi(yg(x))\Big] \tag{29}$$

The empirical Φ-risk is defined as

$$R_{\Phi,n}(g) = \frac{1}{n}\sum_{i=1}^{n}\Phi(y_i g(x_i)) \tag{30}$$

Convex surrogate

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Definition

The Φ-risk is defined as

$$R_\Phi(g) = E\Big[\Phi(yg(x))\Big] \tag{31}$$

The empirical Φ-risk is defined as

$$R_{\Phi,n}(g) = \frac{1}{n}\sum_{i=1}^{n}\Phi(y_i g(x_i)) \tag{32}$$

Key question : does minimizing the Φ-risk lead to a good "0-1" loss prediction ?

Most common convex surrogates

Definition

Logistic loss

$$\Phi(u) = \log(1 + e^{-u}) \tag{33}$$

With linear predictors, this loss will lead to **logistic regression** (which is classification despite its name).

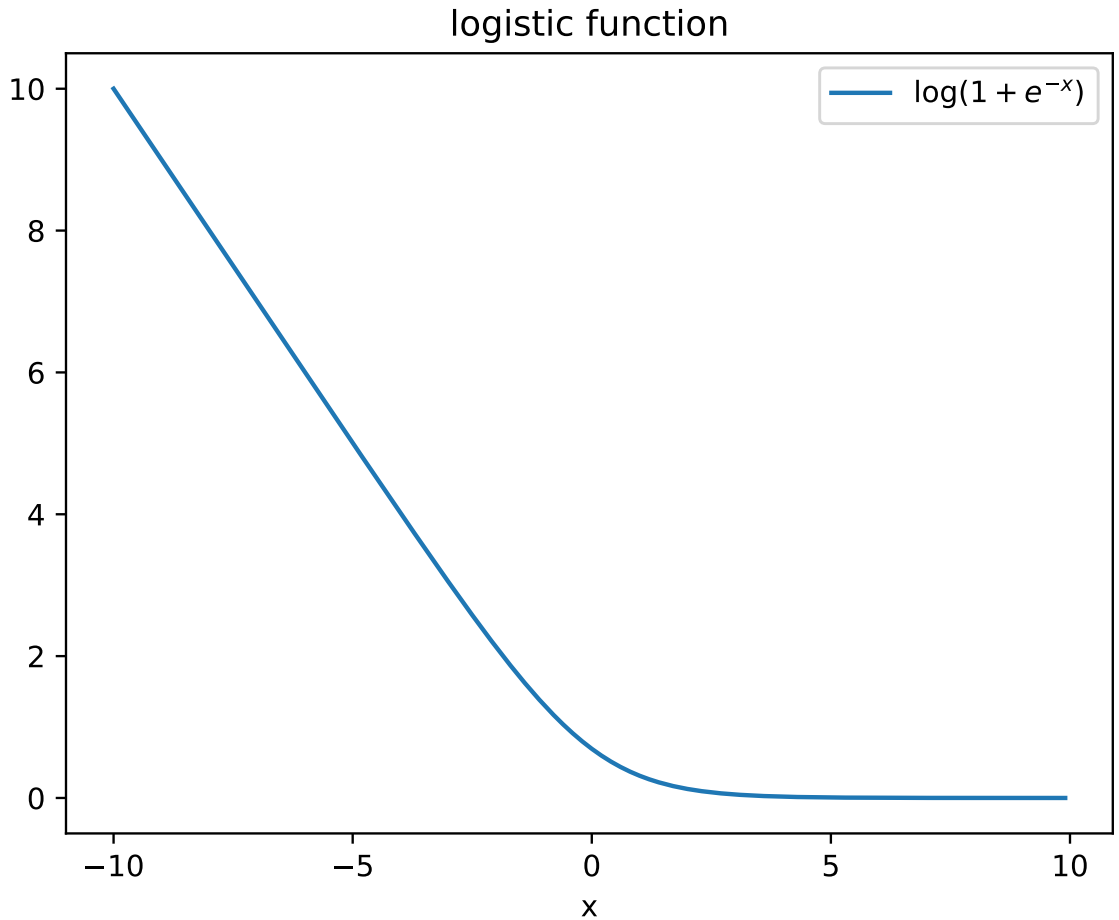
Most common convex surrogates

If $\mathcal{Y} = \{0, 1\}$, $\hat{y}$ is the prediction and y is the correct label, then we sometimes write :

$$l(\hat{y}, y) = y \log(1 + e^{-\hat{y}}) + (1 - y) \log(1 + e^{\hat{y}}) \qquad (34)$$

(cross entropy loss)

Logistic function



Most common convex surrogates

Definition

Hinge loss

$$\Phi(u) = max(1 - u, 0) \tag{35}$$

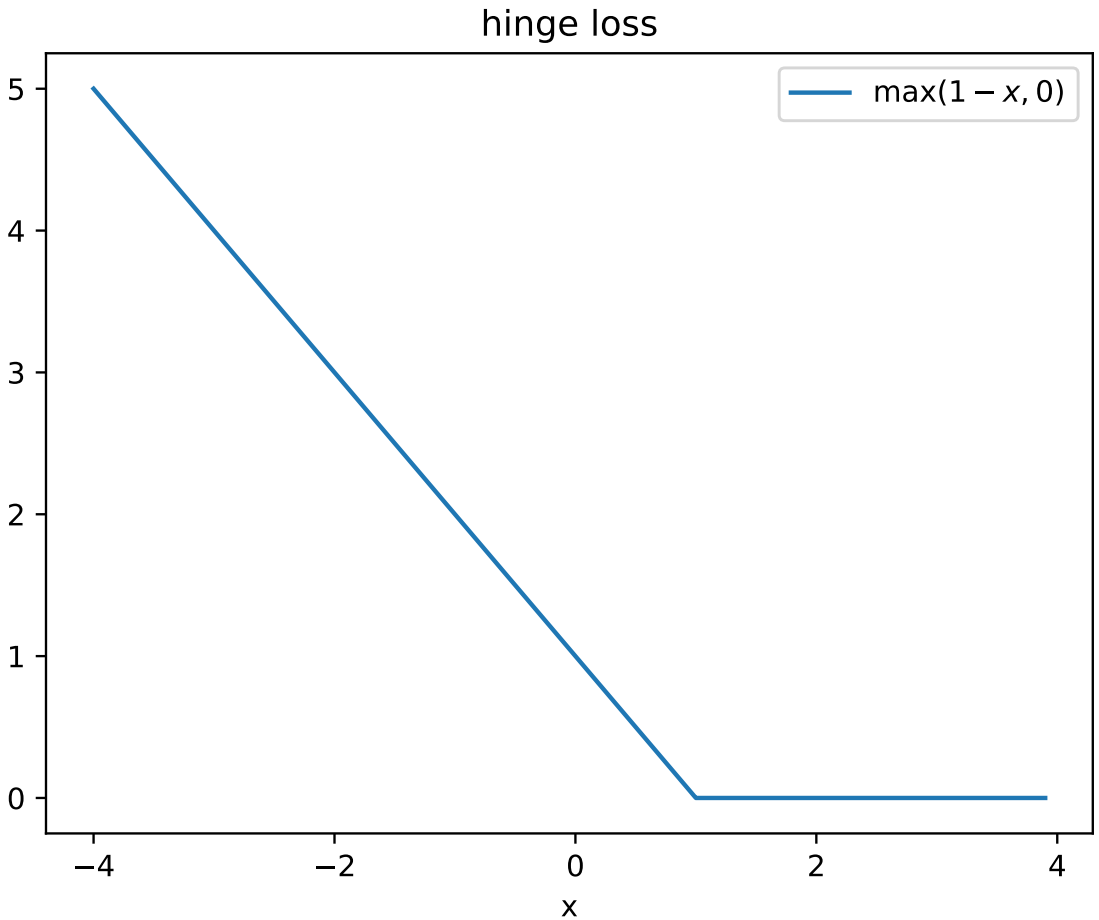
With linear predictors, this loss will lead to **Support vector machines**.

Definition

Squared hinge loss

$$\Phi(u) = (max(1 - u, 0))^2 \tag{36}$$

Hinge loss



Φ-risk minimization

- We come back to the question : does minimizing the empirical Φ-risk lead to a good "0-1" loss prediction ?
- The Bayes predictor stays the same, but several Φ can be used. Hence, several minimizers can be obtained, since the minimizer or the Φ-risk depends on the choice of Φ.

Phi-risk minimization

- Testing error

$$R(g) = E\Big[\Phi_{0-1}(yg(x))\Big] \tag{37}$$

- Testing loss

$$R_\Phi(g) = E\Big[\Phi(yg(x))\Big] \tag{38}$$

Conditional Φ-risk

Definition

Conditional Φ-risk

$$E\Big[\Phi(yg(x))|x\Big] = \eta(x)\Phi(g(x))+(1-\eta(x))\Phi(-g(x)) = C_{\eta(x)}(g(x)) \tag{39}$$

with

$$C_\eta(\alpha) = \eta\Phi(\alpha) + (1-\eta)\Phi(-\alpha) \tag{40}$$

Calibrated Φ

We say that Φ is *calibrated* if :

- $\eta > \frac{1}{2} \Leftrightarrow \arg\min_{\alpha \in \mathbb{R}} C_\eta(\alpha) \subset \mathbb{R}_+^*$
- $\eta < \frac{1}{2} \Leftrightarrow \arg\min_{\alpha \in \mathbb{R}} C_\eta(\alpha) \subset \mathbb{R}_-^*$

This means that the optimal $\forall x$, taken independently, the optimal $g(x)$ obtained by minimizing the conditional Φ-risk leads to the same prediction as the Bayes predictor.

Necessary and sufficient condition

Proposition

Let $\Phi : \mathbb{R} \to \mathbb{R}$ *convex.*

Φ *is calibrated* $\Leftrightarrow$ Φ *is differentiable at* 0 *and* $\Phi'(0) < 0$.

Necessary and sufficient condition

Proposition

Let $\Phi : \mathbb{R} \to \mathbb{R}$ *convex.*
Φ *is calibrated* $\Leftrightarrow$ Φ *is differentiable at* 0 *and* $\Phi'(0) < 0$.

The conditions are verified for the logistic loss and the hinge loss.

Calibration function

To know if minimizing $R_\Phi(g)$ leads to minimizing $R(g)$, it would be sufficient to have a monotonic function H (calibration function), such that

$$R(g) - R^* \leq H\left[R_\Phi(g) - R_\Phi^*\right] \tag{41}$$

Logistic regression

- $g(x) = \langle x, \theta \rangle = x^T \theta$.
- $f(x) = \text{sign}(\langle x^T \theta \rangle)$
- It can be seen as "linear regression applied to classification".

Logistic regression

In this section we use the setting $\mathcal{Y} = \{0, 1\}$.

- prediction : $\hat{y} = x^T \theta$

$$l(\hat{y}, y) = y \log(1 + e^{-\hat{y}}) + (1 - y) \log(1 + e^{\hat{y}}) \qquad (42)$$

(cross entropy loss)

Logistic regression estimator

If l is the logistic loss, it is defined as

$$\hat{\theta}_{logit} = \arg\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} l(x_i^T \theta, y_i)$$

Logistic regression

Exercice 5 : **Convexity**

Show that the logistic loss is stricly convex in θ :

$$\theta \mapsto y \log(1 + e^{-x^T \theta}) + (1 - y) \log(1 + e^{x^T \theta}) \tag{43}$$

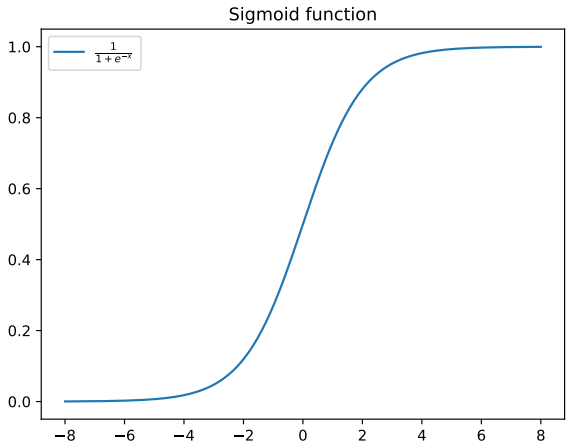
Sigmoid

Definition

Sigmoid function

$\sigma : \mathbb{R} \to \mathbb{R}$.

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{44}$$



No closed-form solution

Since the loss is convex, to minimize it is sufficient to look for the cancellation of the gradient. However, the corresponding equation has no closed-form solution.
We thus need to use iterative algorithms (Gradient descent, Newton's method)

Practical usage of logistic regression

In practice, it is common practice to :

- regularize the logistic loss to avoid overfitting, for instance with a $L2$ penalty (as in ridge regression)
- use feature maps and classify with $\phi(x)$ instead of x.

Likelihood

Let $\mathcal{P} = \{p_\theta, \theta \in \Theta\}$ be a parametric model. Given $y \in \mathcal{Y}$, the **likelihood** of θ is defined as the function $\theta \mapsto p_\theta(y)$.
The likelihood $L(.|D_n)$ of a dataset $D_n = (y_1, \ldots, y_n)$ is defined as

$$L(.|D_n) : \theta \mapsto \prod_{i=1}^{n} p_\theta(y_i)$$

Likelihood

Since the samples y_i are assumed to be independent, the likelihood corresponds to the probability of observing the dataset according to p_θ. We can define a loss function as the **negative log-likelihood.**

$$\Theta \times \mathcal{Y} \mapsto -\log(p_\theta(y))$$

Given this loss, the risk writes :

$$R(\theta) = E_Y[-\log\left(p_\theta(y)\right)]$$

and the empirical risk (ER) :

$$R_n(\theta) = -\frac{1}{n}\sum_{i=1}^{n} \log\left(p_\theta(y_i)\right)]$$

Maximum likelihood

Finding the parameter with maximum likelihood means finding the parameter that minimizes $R_n(\theta)$.

$$R_n(\theta) = -\frac{1}{n}\sum_{i=1}^{n} \log\left(p_\theta(y_i)\right)]$$

Link with logistic regression

Let us now consider the probabilistic model such that

$$p_\theta(1|x) = \sigma(\theta^T x)$$

which makes sense since $\sigma(\theta^T x) \in [0, 1]$, and can thus be interpreted as a probability.

Link with logistic regression

Let us now consider the probabilistic model such that

$$p_\theta(1|x) = \sigma(\theta^T x)$$

which makes sense since $\sigma(\theta^T x) \in [0, 1]$, and can thus be interpreted as a probability.
Equivalently, this model can be written (remember that $y = 0$ or $y = 1$)

$$p_\theta(y|x) = \left(\sigma(\theta^T x)\right)^y \left(1 - \sigma(\theta^T x)\right)^{1-y}$$

Link with logistic regression

Let us now consider the probabilistic model such that

$$p_\theta(1|x) = \sigma(\theta^T x)$$

We will show that the parameter θ with maximum likelihood is the logistic regression estimator θ_{logit}.

$$
\begin{aligned}
R_n(\theta) &= -\frac{1}{n}\sum_{i=1}^{n} \log\left(p_\theta(y_i|x_i)\right) \\
&= -\frac{1}{n}\sum_{i=1}^{n} \log\left(\left(\sigma(\theta^T x_i)\right)_i^y \left(1-\sigma(\theta^T x_i)\right)^{1-y_i}\right) \\
&= -\frac{1}{n}\sum_{i=1}^{n} y_i \log\left(\sigma(\theta^T x_i)\right) + (1-y_i)\log\left(\sigma(-\theta^T x_i)\right) \\
&= \frac{1}{n}\sum_{i=1}^{n} y_i \log\left(1+e^{\theta^T x_i}\right) + (1-y_i)\log\left(1-e^{\theta^T x_i}\right) \\
&= \frac{1}{n}\sum_{i=1}^{n} l(\theta^T x_i, y_i)
\end{aligned}
$$

Empirical risk minimization for the log-likelihood with this model and the logistic regression are the same.