Machine learning I, supervised learning: logistic regression

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 1 : **Combinatorial problem**
If we wanted to try all mappings in $\mathcal{Y}^{\mathcal{X}}$, if $|\mathcal{X}| = n$, how many mappings would there be ?

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 $f = \text{sign} \circ g$ writes :

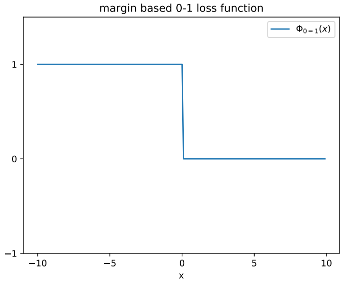
$$\begin{aligned} R(g) &= P(\text{sign}(g(x)) \neq y) \\ &= E\left[1_{\text{sign}(g(x)) \neq y}\right] \\ &= E\left[1_{yg(x)<0}\right] \end{aligned} \tag{1}$$

Several solutions

There might be many optimal maps g, i.e : such that $\text{sign}(g(x)) = f^*(x)$ for all x.
(Here, $f^*(x)$ is the Bayes predictor, which is the optimal predictor : it minimizes the generalization error (risque réel))

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

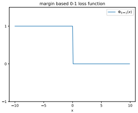
$$
\begin{aligned}
R(g) &= E\left[1_{\text{sign}(g(x))\neq y}\right] \\
&= E\left[1_{yg(x)<0}\right] \\
&= E\left[\Phi_{0-1}(yg(x))\right]
\end{aligned}
\tag{2}
$$



Empirical risk minimization

The corresponding empirical risk writes :

$$\frac{1}{n}\sum_{i=1}^{n}\Phi_{0-1}(y_i g(x_i)) \tag{3}$$



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.
Natural question : but does minimizing the Φ-risk lead to a good "0-1" loss prediction ? Answering this question requires an advanced study.

Most common convex surrogates

Définition

Logistic loss

$$\Phi(u) = \log(1 + e^{-u}) \tag{4}$$

With linear predictors ($g(x_i) = \langle \theta, x_i \rangle$), this loss will lead to **logistic regression** (which is classification despite its name).

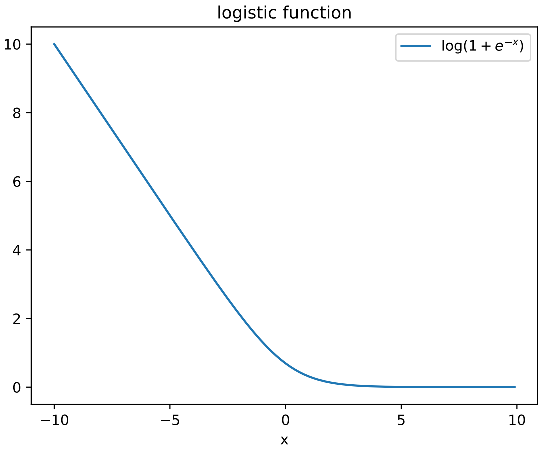
Most common convex surrogates

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

$$l(\hat{y}, y) = y \log(1 + e^{-\hat{y}}) + (1 - y) \log(1 + e^{\hat{y}}) \tag{5}$$

(cross entropy loss)

Logistic function



Most common convex surrogates

Définition

Hinge loss

$$\Phi(u) = max(1 - u, 0) \tag{6}$$

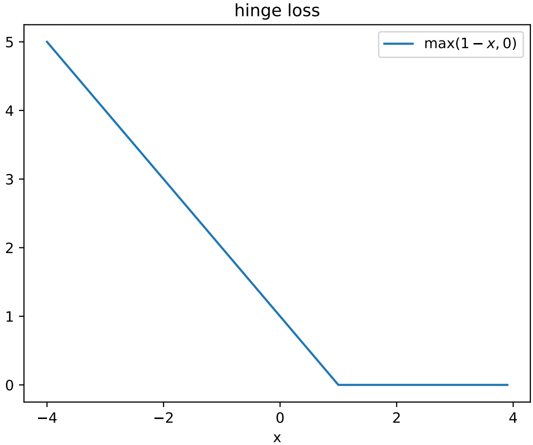
With linear predictors, this loss will lead to **Support vector machines**.

Définition

Squared hinge loss

$$\Phi(u) = (max(1 - u, 0))^2 \tag{7}$$

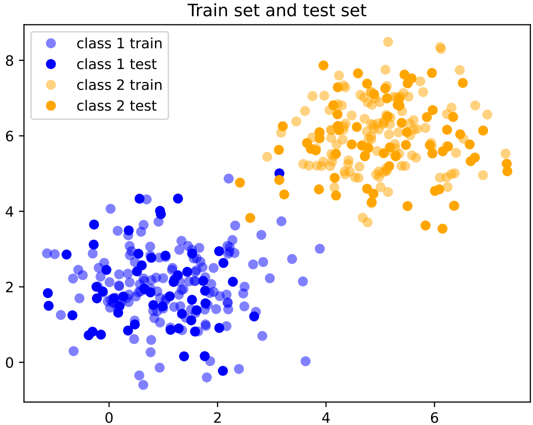
Hinge loss



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".

Application on a toy dataset



Application on a toy dataset

Logistic regression

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

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

$$l(\hat{y}, y) = y \log(1 + e^{-\hat{y}}) + (1 - y) \log(1 + e^{\hat{y}}) \tag{8}$$

(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

We can show that the logistic loss is stricly convex in θ :

$$\theta \mapsto y \log(1 + e^{-x^T\theta}) + (1 - y) \log(1 + e^{x^T\theta}) \tag{9}$$

This means that if we manage to fing θ that cancels the **gradient** of the empirical risk, θ is a global minimizer.

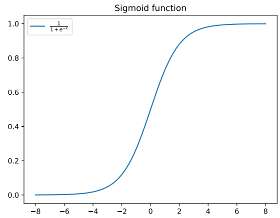
Sigmoid

Définition

Sigmoid function

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

$$\sigma(x) = \frac{1}{1+e^{-x}} \tag{10}$$



No closed-form solution

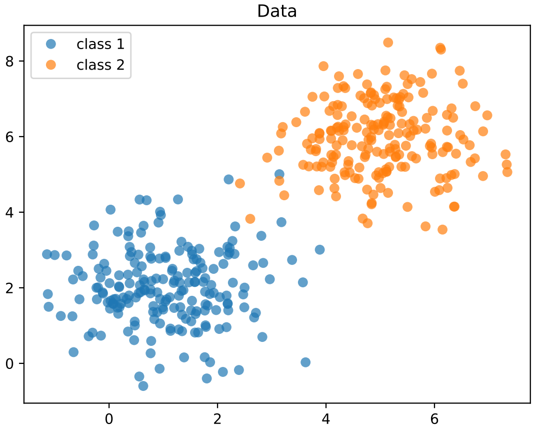
Since the loss is convex, to minimize it is sufficient to look for the cancellation of the gradient. However, the corresponding equation has no closed-form solution.
We thus need to use iterative algorithms (Gradient descent, Newton's method)

Practical usage of logistic regression

In practice, it is common practice to :

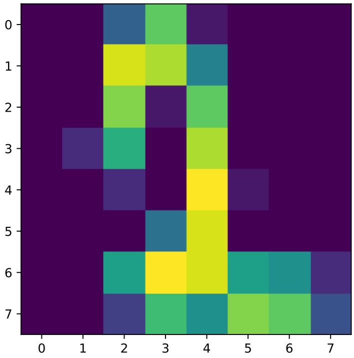
- regularize the logistic loss to avoid overfitting, for instance with a $L2$ penalty (as in ridge regression)
- use feature maps and classify with $\phi(x)$ instead of x.

Application to a simple 2D dataset.



Application to the digits dataset.

https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_digits.html



Data transformation (feature maps)