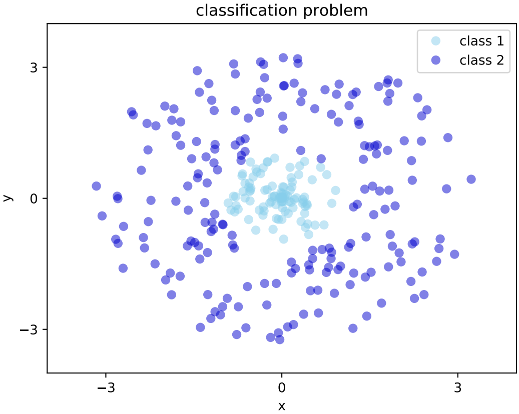
Fondamentaux théoriques du machine learning



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

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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

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

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

The equation of the cancellation of the gradient is

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

which we can write

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

$\hat{\Sigma} + 2\lambda I_d$ 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.

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

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Maximum likelihood

Feature maps

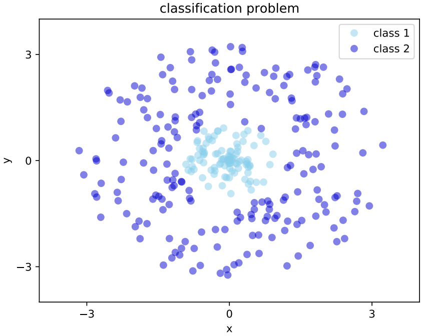
Often, we do not work with the $x_i \in \mathcal{X}$, but with **representations** $\phi(x_i)$, with $\phi : \mathcal{X} \to \mathbb{R}^d$. Possible motivations :

- $\mathcal{X}$ 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.

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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

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

$E\big(l(X,Y)|X\big)$ is the expectation of $l(X,Y)$ given X.

Bayes predictor

Hence,

$$f^*(x) = \underset{z \in \mathcal{Y}}{\arg\min}\, E\left[l(y, z) | X = x\right] \tag{18}$$

Bayes predictor

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

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

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

Bayes risk

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

Bayes risk

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

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 $p = 1/3$, $q = 3/4$.

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

$$Y = \left\{ \begin{array}{l} B(1/3) \text{ if } X = 1 \\ B(3/4) \text{ if } X = 0 \end{array} \right.$$

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

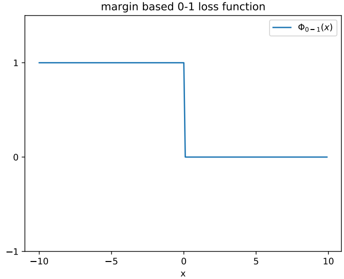
$$\begin{aligned} R(g) &= P(\text{sign}(g(x)) \neq y) \\ &= E\left[1_{\text{sign}(g(x)) \neq y}\right] \\ &= E\left[1_{yg(x) < 0}\right] \end{aligned} \tag{25}$$

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}

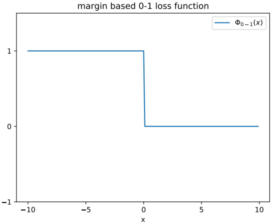
$$\begin{aligned} R(g) &= E\left[1_{\text{sign}(g(x)) \neq y}\right] \\ &= E\left[1_{yg(x)<0}\right] \\ &= E\left[\Phi_{0-1}(yg(x))\right] \end{aligned} \tag{26}$$



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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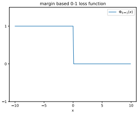

What is the issue with this objective function ?

- 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).

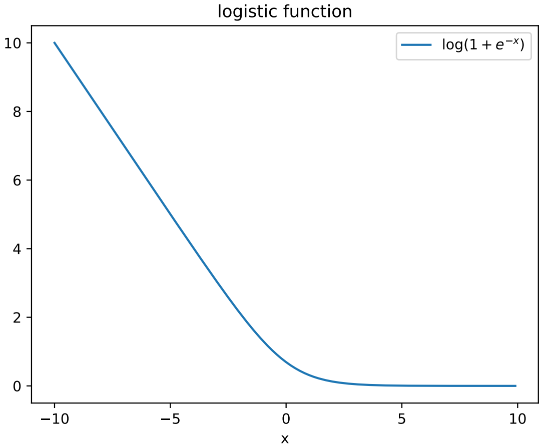
Most common convex surrogates

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

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

(cross entropy loss)

Logistic function



Most common convex surrogates

Definition

Hinge loss

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

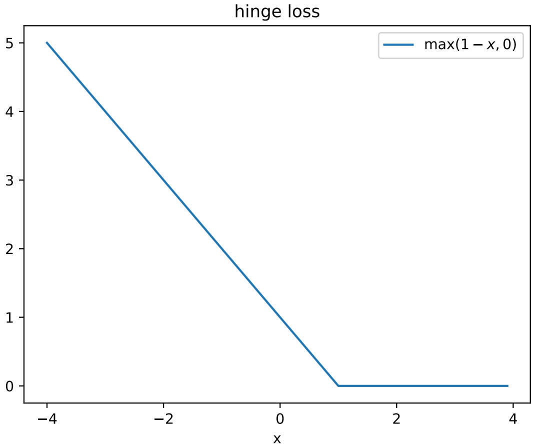
With linear predictors, this loss will lead to **Support vector machines**.

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

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

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

Necessary and sufficient condition

Proposition

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

Φ *is calibrated* $\Leftrightarrow \Phi$ *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

$$R(g) - R^* \leq H\Big[R_\Phi(g) - R_\Phi^*\Big] \qquad (41)$$

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

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

(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 :

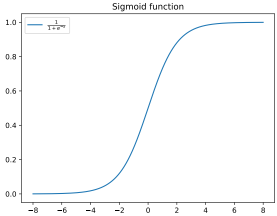
$$\theta \mapsto y\log(1+e^{-x^T\theta}) + (1-y)\log(1+e^{x^T\theta}) \tag{43}$$

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 $D_n = (y_1, \dots, y_n)$ 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 $R_n(\theta)$.

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

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

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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}.

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

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