Advanced Machine Learning

Lecture 2: Robust Regression

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CentraleSupélec

Content

Today's Lecture

1. Reminders
    1. Linear Regression
    2. Regularized regression

2. Robust regression
    1. M-estimation
    2. The IRLS algorithm

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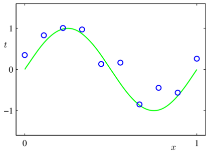
Regression: A supervised approach

- Let $\boldsymbol{X} = (x_1, ..., x_n)$ and $\boldsymbol{Y} = (y_1, ..., y_n)$ be a set of $\boldsymbol{n}$ input/ouput training samples.
- Estimate/learn a prediction function $y = f(x)$
- $\boldsymbol{Y}$ known : supervised

Regression

- $y \in \mathbb{R}$ is a continuous variable
- Predict a numerical value



Applications

Stock price prediction, weather forecast, ...

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Linear Regression: Motivations

- Simple approach (essential to understand more sophisticated ones)
- Interpretable description of the relations inputs/outputs
- Can outperform nonlinear models, in the case of few training data/high noise/sparse data
- Extended applicability when combined with basis-function methods (see Lab)

Linear Regression: Applications

- Future product sales based on purchase history/client behaviour
- Economic growth of a country
- Housing market prediction: in a few months, at what price?
- Number of goals a player will score in the coming matches based on previous performance
- Hours of study needed to pass a test

Linear regression: Problem Formulation

Using the training set, learn the linear function $\boldsymbol{f}_\beta$ (parametrized by $\boldsymbol{\beta}$) predicting a real value $\boldsymbol{y} \in \mathbb{R}$ from an observation $\boldsymbol{x}_i \in \mathbb{R}^d$:

$$y_i \approx f_\beta(\boldsymbol{x}_i), \quad \forall i \in \{1, .., n\}$$

Fitting model

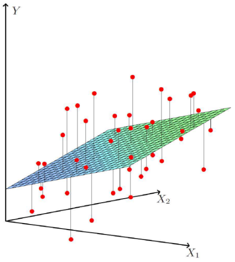
$$f_\beta(\boldsymbol{x}_i) = \beta_0 1 + \beta_1 \boldsymbol{x}_{i,1} + ... + \beta_d \boldsymbol{x}_{i,d} = \boldsymbol{x'}_i{}^T \boldsymbol{\beta} = [\boldsymbol{X}\beta]_i$$

- $\boldsymbol{X} \in \mathbb{R}^{n \times d+1}$ with $\boldsymbol{x'}_i = [1, \boldsymbol{x}_{i,1}, ..., \boldsymbol{x}_{i,d}]$ its ith line
- $\boldsymbol{\beta} = [\beta_1, ..., \beta_d]$ defines a hyperplan in $\mathbb{R}^d$
- $\boldsymbol{\beta}_0$ can be viewed as a bias that shifts the function $\boldsymbol{f}$ perpendicularly to the hyperplan

Least Squares

Find β minimizing the sum of squared residuals $\mathbf{e} = \boldsymbol{X}\beta - \boldsymbol{y}$

$$L(\beta) = \frac{1}{2}\sum_{i=1}^{n}[y_i - f(\boldsymbol{x}_i)]^2 = \frac{1}{2}\|\boldsymbol{X}\beta - \boldsymbol{y}\|^2 = \frac{1}{2}\|\mathbf{e}\|^2$$



Solution $\rightarrow$ equate the gradient to zero

Least Squares Solution

Solve $\min_{\boldsymbol{\beta}} L(\boldsymbol{\beta})$ where $L : \mathbb{R}^{d+1} \to \mathbb{R}$ is convex

$$\hat{\beta} \text{ minimizer of } L \iff \nabla L(\hat{\beta}) = 0$$

where

$$[\nabla L(\boldsymbol{\beta})]_j = \frac{\partial L(\beta)}{\partial \beta_j}, \ \forall j \in 1, .., d$$

How do we compute the solution?

- $L(\boldsymbol{\beta}) = \frac{1}{2}\|\boldsymbol{X}\beta - \boldsymbol{y}\|^2 = \frac{1}{2}\boldsymbol{y}^T\boldsymbol{y} - \beta^T\boldsymbol{X}^T\boldsymbol{y} + \frac{1}{2}\beta^T\boldsymbol{X}^T\boldsymbol{X}\beta$
- $\nabla L(\boldsymbol{\beta}) = -\boldsymbol{X}^T\boldsymbol{y} + \boldsymbol{X}^T\beta$

If $\boldsymbol{X}$ is full column rank then $\boldsymbol{X}^T\boldsymbol{X}$ is positive definite, the solution is unique and

$$\hat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

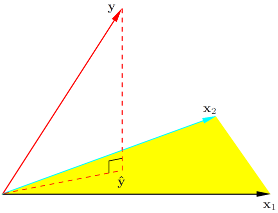
White board

Interpretation of the LS solution

We obtain the fitted values for the training inputs

$$y = \boldsymbol{X}\beta = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y}$$

- $\boldsymbol{H}$ is called the *hat matrix* and computes the orthogonal projection of $\boldsymbol{y}$ onto the vectorial subspace spanned by the columns of $\boldsymbol{X}$.



Statistical properties

For uncorrelated observations $\boldsymbol{y}_i$ with variance σ^2, and deterministic $\mathbf{x}_i$

$$\mathrm{Var}(\hat{\beta}) = (\mathbf{X}^\top \mathbf{X})^{-1}\sigma^2$$

Unbiased estimator:

$$\hat{\sigma}^2 = \frac{1}{n-(d+1)} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Inference properties

Assume that $Y = \beta_0 + \sum_{j=1}^{d} X_j \beta_j + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \sigma^2)$. Then $\hat{\beta}$ and $\hat{\sigma}$ are independant and

- $\hat{\beta} \sim \mathcal{N}(\beta, (\mathbf{X}^\top \mathbf{X})^{-1}\sigma^2)$
- $(n-(d+1))\hat{\sigma}^2 \sim \sigma^2 \chi^2_{n-(d+1)}$

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High dimensional linear regression

Some problems arise with least squares regression when d is large

- Accuracy: The hyperplan fits the data well but predicts/generalizes badly. (low bias / large variance)
- Interpretation: Identify a small subset of features important/relevant for predicting the data.

High dimensional linear regression

Some problems arise with least squares regression when d is large

- Accuracy: The hyperplan fits the data well but predicts/generalizes badly. (low bias / large variance)
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How can we tackle the above issues ?

Use an additional regularization term $R(\beta)$

$$L(\beta) = \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda R(\beta)$$

Common regularization types

Ridge regression

Reduces the magnitudes of the coefficients in β

$$R(\beta) = \frac{1}{2}\|\beta\|^2$$ Explicit solution!

Shrinkage

Sparsifies the coefficients in β : most elements are zero

$$R(\beta) = \|\beta\|_1$$ Optimization method needed!

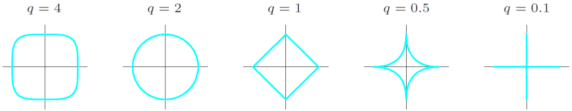
Subset selection

Sparsifies the coefficients in β : most elements are zero

$$R(\beta) = \|\beta\|_0$$ Optimization method needed!

White board

Penalty functions



Contour plots for $\sum_j |\beta_j|^q$

When the columns of $\mathbf{X}$ are orthonormal, the estimators can be deduced from the LS estimator $\hat{\beta}$ according to:

- Ridge : $\hat{\beta}_j/(1+\lambda)$ weight decay
- Lasso : $\text{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda)_+$ soft tresholding
- Best subset : $\hat{\beta}_j \cdot \delta\left(\hat{\beta}_j^2 \geq 2\lambda\right)$ hard tresholding

Proximal Gradient

- Gradient step

$$\bar{\beta}_k = \beta_k - \theta \nabla L(\beta_k)$$

- Proximal gradient step

$$\beta_{k+1} = \underset{\beta}{argmin} \frac{1}{2} \|\bar{\beta}_k - \beta\|^2 + \lambda \theta R(\beta)$$

- Guarantied convergence to a local minimum when $\theta \in]0, \frac{2}{\|X^T X\|}[$
- $F(\beta_k)$ will decrease monotonicallly with k
- Global minimum with ℓ_1 norm
- Local minimum with the non-convex ℓ_0-norm

Solutions for the proximal step

- $R(\beta) = \|\beta\|_1$

$$\beta_{k+1} = sign(\bar{\beta}_k) \times max(|\bar{\beta}_k| - \lambda\theta, 0)$$

- $R(\beta) = \|\beta\|_0$

$$\beta_{k+1} = \bar{\beta}_k \times \delta(\bar{\beta}_k^2 \leq 2\lambda\theta)$$

Element-wise operations!

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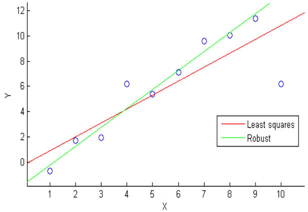
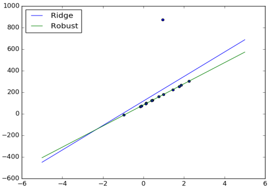
Least Squares shortcomings

What happens in the presence of outliers ?

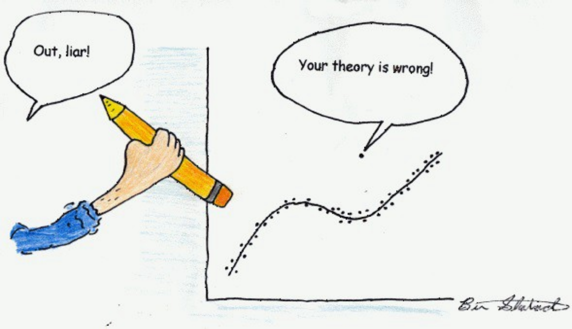




Different problems can be adressed

- Outliers in the dataset
- Mismodelling of the data set

Robust Statistics



Goal

Design estimation methods insensitive to outliers and possibly high leverage points

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Robust Statistics: M-estimation

Maximum Likelihood-type estimates

One-Parameter Case: $X_1, ..., X_n$ i.i.d. $\sim f(x;\theta), \theta \in \Theta$

- Likelihood function: $L(x_1, ..., x_n; \theta) = \prod_{i=1}^{n} f(x_i; \theta)$
- Minimize the negative log-likelihood:

$$\min_{\theta} \sum_{i=1}^{n} \rho(x_i; \theta) \text{ where } \rho(x; \theta) = -\log f(x; \theta).$$

- Solve the likelihood equations:

$$\sum_{i=1}^{n} \psi(x_i; \theta) = 0 \text{ where } \psi(x_i; \theta) = \frac{\partial \rho(x_i; \theta)}{\partial \theta}$$

Robust regression: Objective function approach

We can achieve robustness using M-estimation

$$L(\beta) = \sum_{i=1}^{n} \rho(y_i - \mathbf{x}_i'^\top \beta)$$

with ρ a potential function satisfying:

- $\rho(e) \geq 0$ and $\rho(0) = 0$
- $\rho(e) = \rho(-e)$
- $\rho(e) \geq \rho(e')$ for $|e| \geq |e'|$

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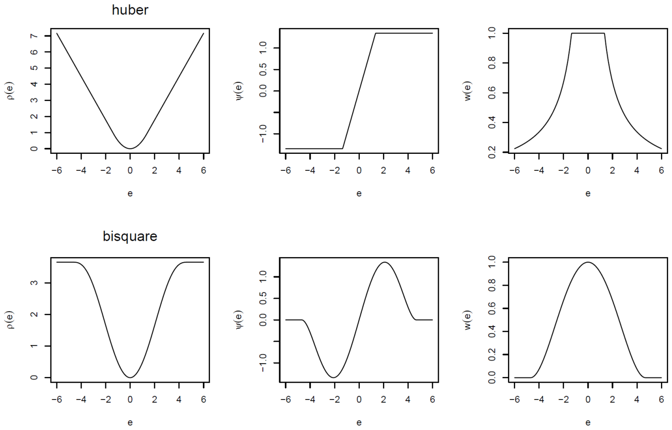
Minimizer satisfies

$$\dot{\rho}(y_i - \mathbf{x}_i'^\top \hat{\beta})\mathbf{x}_i' = 0, \quad i = 1, \ldots, n$$

$\rightarrow$ IRLS algorithm

Examples of functions ρ



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IRLS : Iteratively Reweighted Least Squares

Key Idea: Iteratively down-weight outliers using information about the errors, *i.e.*,
The largest errors at step $k-1$ ($\mathbf{e}^k = \boldsymbol{X}\hat{\beta}^k - \mathbf{y}$) are assigned low weights $\boldsymbol{W}^k$ at the current step k

- The weights are computed using a weight function (based on ρ)

$$\omega(e_i) = \frac{\dot{\rho}(e_i)}{e_i}, \ \forall i = 1, ..., n$$

- Recall that the minimizer $\hat{\beta}$ satisfies

$$\dot{\rho}(y_i - \mathbf{x}_i'^{\top}\hat{\beta})\mathbf{x}_i' = 0, \quad i = 1, \dots, n \qquad (1)$$

$$\omega(e_i)e_i\frac{\partial e_i}{\partial \beta_j} = 0, \quad j = 1, \dots, d \qquad (2)$$

- (2) corresponds to solving:
  min $\sum_{i=1}^{n} \omega(e_i^{k-1})e_i^2$ (or min $\|\boldsymbol{W}_{k-1}^{\frac{1}{2}}(\boldsymbol{X}\hat{\beta}_k - \mathbf{y})\|^2$)

IRLS algorithm: Majorization-Minimization approach

Let ρ be defined as

$$(\forall x \in \mathbb{R}) \qquad \rho(x) = \phi(|x|)$$

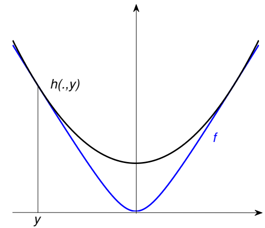
where

(i) ϕ is differentiable on $]0, +\infty[$,

(ii) $\phi(\sqrt{\cdot})$ is concave on $]0, +\infty[$,

(iii) $(\forall x \in [0, +\infty[) \quad \dot{\phi}(x) \geq 0$,

(iv) $\lim_{\substack{x \to 0 \\ x > 0}} \left(\omega(x) := \frac{\dot{\phi}(x)}{x} \right) \in \mathbb{R}$.



Then, for all $y \in \mathbb{R}$,

$$(\forall x \in \mathbb{R}) \quad \rho(x) \leq \rho(y) + \dot{\rho}(y)(x - y) + \frac{1}{2}\omega(|y|)(x - y)^2.$$

Examples of functions ρ

	$\rho(x)$	$\omega(x)$ (exercise)
Convex	$\lvert x\rvert - \delta \log(\lvert x\rvert/\delta + 1)$	
	$\begin{cases} x^2 & \text{if } \lvert x\rvert < \delta \\ 2\delta\lvert x\rvert - \delta^2 & \text{otherwise} \end{cases}$	
	$\log(\cosh(x))$	
	$(1 + x^2/\delta^2)^{\kappa/2} - 1$	
Nonconvex	$1 - \exp(-x^2/(2\delta^2))$	
	$x^2/(2\delta^2 + x^2)$	
	$\begin{cases} 1 - (1 - x^2/(6\delta^2))^3 & \text{if } \lvert x\rvert \leq \sqrt{6}\delta \\ 1 & \text{otherwise} \end{cases}$	
	$\tanh(x^2/(2\delta^2))$	
	$\log(1 + x^2/\delta^2)$	

$$(\lambda, \delta) \in]0, +\infty[^2,\ \kappa \in [1, 2]$$

White board

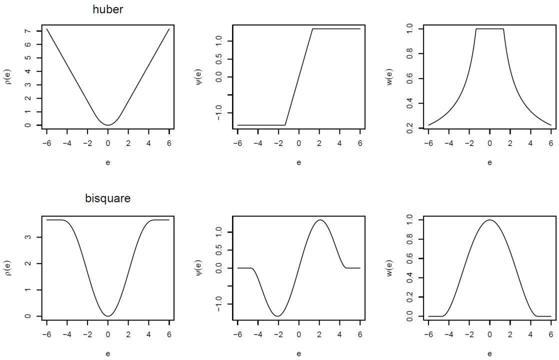
IRLS algorithm

The IRLS weight matrix is

$$\mathbf{W}_k = \mathrm{Diag}(\omega(\mathbf{y} - \mathbf{X}\beta_k))$$

and

$$(\forall k \in \mathcal{N}) \quad \beta_{k+1} = (\mathbf{X}^\top \mathbf{W}_k \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{W}_k \mathbf{y}.$$



IRLS algorithm: Summary

Algorithm

- Initialize $\boldsymbol{\beta}_0$ (e.g., LS estimates)
- Then iterate between the following steps:

For $k = 1, ..., k_{max}$

1. Compute $\boldsymbol{e}^{k-1} = \boldsymbol{Y} - \boldsymbol{X}^T \boldsymbol{\beta}_{k-1}$
2. Compute $\boldsymbol{W}_k = diag[\omega(e_i^{k-1})]$
3. Update the estimate $\boldsymbol{\beta}_k = (\mathbf{X}^\top \mathbf{W}_k \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{W}_k \mathbf{y}$