Session 10: Linear regression

Optimization and Computational Linear Algebra for Data Science

Marylou Gabrié (based on material by Léo Miolane)

Contents

Introduction

- We have n « feature vectors » $a_1, \dots, a_n \in \mathbb{R}^d$.
- Each point a_i comes with a « target variable » $y_i \in \mathbb{R}$.
- **Goal.** Find a linear relation between the a_is and the y_is:

- **Prediction:**

Can we have an intercept?

Find $x \in \mathbb{R}^d$ such that $y_i = \langle x, a_i \rangle + \mathbf{c}$.

Solving $Ax = y$ is a bad idea

The system $Ax = y$ may have:

- No solution.

- Infinitely many solutions.

1. Ordinary least squares

Least squares problem

(LS) Minimize $f(x) = \|Ax - y\|^2$ with respect to $x \in \mathbb{R}^d$.

The Moore-Penrose pseudo-inverse

What if $A^\top A$ is not invertible?

Definition

Let $A = U\Sigma V^\mathsf{T}$ be the SVD of A. The matrix $A^\dagger \stackrel{\text{def}}{=} V\Sigma' U^\mathsf{T}$ is called the **(Moore-Penrose) pseudo-inverse** of A, where $\Sigma' \in \mathbb{R}^{d\times n}$ is

$$\Sigma'_{i,i} = \begin{cases} 1/\Sigma_{i,i} & \text{if } \Sigma_{i,i} \neq 0 \\ 0 & \text{otherwise} \end{cases}, \quad \text{and} \quad \Sigma'_{i,j} = 0 \ \text{ for } \ i \neq j$$

Exercise: Check that if A is invertible then $A^{-1} = A^\dagger$.

Solving $A^{\mathsf{T}}Ax = A^{\mathsf{T}}y$

Claim: The vector $x^{\mathrm{LS}} \stackrel{\mathrm{def}}{=} A^{\dagger}y$ is a solution of $A^{\mathsf{T}}Ax = A^{\mathsf{T}}y$

Theorem

The set of the minimizers of $f(x) = \|Ax - y\|^2$ is

$$\left\{ x^{\mathrm{LS}} + v \,\middle|\, v \in \mathrm{Ker}(A) \right\}.$$

2. Penalized least squares

Ridge regression

Ridge regression consists in adding a « ℓ_2 penalty » :

(Ridge) Minimize $f(x) = \|Ax - y\|^2 + \lambda \|x\|^2$ w.r.t. $x \in \mathbb{R}^d$.

for some fixed $\lambda > 0$.

Lasso

The Lasso adds a « ℓ_1 penalty » :

(Lasso) Minimize $f(x) = \|Ax - y\|^2 + \lambda \|x\|_1$ w.r.t. $x \in \mathbb{R}^d$.

for some fixed $\lambda > 0$.

Intuition behind feature selection

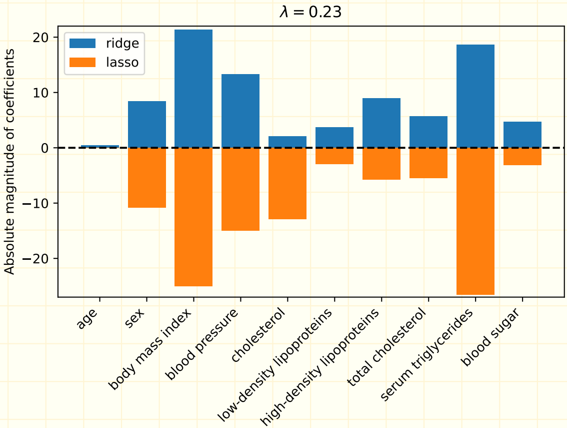
Lemma

Let x^{Lasso} be a minimizer of the Lasso cost function and let $r = \|x^{\text{Lasso}}\|_1$. Then x^{Lasso} is a solution to the constrained optimization problem:

$$\text{minimize} \quad \|Ax - y\|^2 \quad \text{subject to} \quad \|x\|_1 \leq r.$$

Effect of Regularization

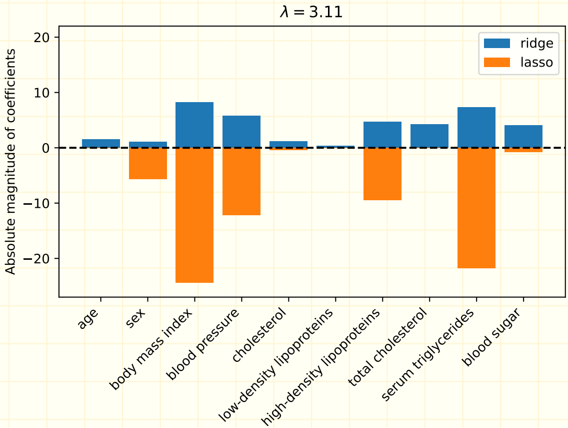
Consider a data set with $n = 442$ patients, with $d = 10$ dimensions feature vectors and the prediction of diabetese disease progression



https://scikit-learn.org/stable/datasets/toy_dataset.html

Effect of Regularization

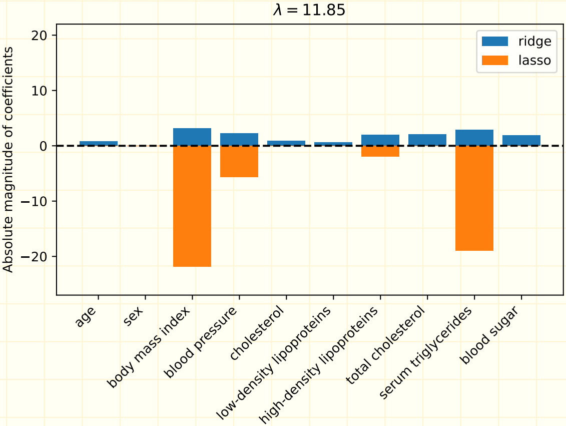
Consider a data set with $n = 442$ patients, with $d = 10$ dimensions feature vectors and the prediction of diabetese disease progression



https://scikit-learn.org/stable/datasets/toy_dataset.html

Effect of Regularization

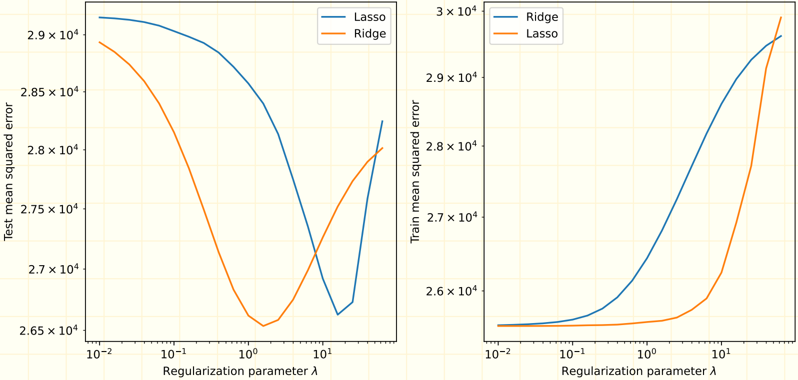
Consider a data set with $n = 442$ patients, with $d = 10$ dimensions feature vectors and the prediction of diabetese disease progression



https://scikit-learn.org/stable/datasets/toy_dataset.html

Effect of Regularization

Consider a data set with $n = 442$ patients, with $d = 10$ dimensions feature vectors and the prediction of diabetese disease progression



`https://scikit-learn.org/stable/datasets/toy_dataset.html`

3. Matrix norms

Frobenius norm

Definition

The Frobenius norm of a matrix $A \in \mathbb{R}^{n \times m}$ is defined as

$$\|A\|_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{m} A_{i,j}^2}$$

Proposition

$$\|A\|_F = \sqrt{\sum_{i=1}^{\min(n,m)} \sigma_i(A)^2}$$

The spectral norm

Definition

The spectral norm of a matrix $A \in \mathbb{R}^{n \times m}$ is defined as

$$\|A\|_{\mathrm{Sp}} = \max_{\|x\|=1} \|Ax\|.$$

Proposition

$$\|A\|_{\mathrm{Sp}} = \sigma_1(A).$$

The nuclear norm

Definition

The nuclear norm of a matrix $A \in \mathbb{R}^{n \times m}$ is defined as

$$\|A\|_\star = \sum_{i=1}^{\min(n,m)} \sigma_i(A).$$

Application to matrix completion

We have a data matrix $M \in \mathbb{R}^{n \times m}$ that we only observe partially. That is we only have access to

$$M_{i,j} \quad \text{for } (i,j) \in \Omega,$$

where $\Omega \subset \{1, \dots, n\} \times \{1, \dots m\}$ is a subset of the complete set of the entries.

Application to matrix completion

Questions?

Questions?