Multivariate Statistics

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Introduction

Definition 1: Long Term Nonprocessor (LTNP)

Patient who will remain a long time in good health condition, even with a large viral load (cf. HIV).

(1) Example 1: Genotype: Qualitative or Quantitative?

$$SNP: \begin{cases} AA \\ AB \end{cases} \rightarrow \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix},$$

thus we might consider genotype either as a qualitative variable or quantitative variable.

When the variable are quantitative, we use regression, whereas for qualitative variables, we use an analysis of variance.

Part I.

1.1. Generalized Linear Model

$$g(\mathbb{E}(Y)) = X\beta$$

with g being

- Logistic regression: $g(v) = \log\left(\frac{v}{1-v}\right)$, for instance for boolean values,
- Poission regression: $g(v) = \log(v)$, for instance for discrete variables.

1.1.1. Penalized Regression

When the number of variables is large, e.g, when the number of explanatory variable is above the number of observations, if p >> n (p: the number of explanatory variable, n is the number of observations), we cannot estimate the parameters. In order to estimate the parameters, we can use penalties (additional terms).

Lasso regression, Elastic Net, etc.

1.1.2. Simple Linear Model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

1.1.3. Assumptions

1.1.4. Statistical Analysis Workflow

Step 1. Graphical representation;

Step 2. ...

$$Y = X\beta + \varepsilon$$
.

is noted equivalently as

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ 1 & x_{31} & x_{32} \\ 1 & x_{41} & x_{42} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{pmatrix}.$$

1.2. Parameter Estimation

1.2.1. Simple Linear Regression

1.2.2. General Case

If $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ is invertible, the OLS estimator is:

$$\hat{\beta} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{Y} \tag{1.1}$$

1.2.3. Ordinary Least Square Algorithm

We want to minimize the distance between $X\beta$ and Y:

$$\min \|\mathbf{Y} - \mathbf{X}\beta\|^2$$

(See chapter 2).

$$\Rightarrow \mathbf{X}\beta = proj^{(1,\mathbf{X})}\mathbf{Y}$$

$$\Rightarrow \forall v \in w, \ vy = vproj^w(y)$$

$$\Rightarrow \forall i :$$

$$\mathbf{X}_i\mathbf{Y} = \mathbf{X}_iX\hat{\beta} \quad \text{where } \hat{\beta} \text{ is the estimator of } \beta$$

$$\Rightarrow \mathbf{X}^T\mathbf{Y} = \mathbf{X}^T\mathbf{X}\hat{\beta}$$

$$\Rightarrow (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X})\hat{\beta}$$

$$\Rightarrow \hat{\beta} = (X^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

This formula comes from the orthogonal projection of \mathbf{Y} on the subspace define by the explanatory variables \mathbf{X}

 $\mathbf{X}\hat{\beta}$ is the closest point to Y in the subspace generated by X.

If H is the projection matrix of the subspace generated by \mathbf{X} , $X\mathbf{Y}$ is the projection on \mathbf{Y} on this subspace, that corresponds to $\mathbf{X}\hat{\beta}$.

1.3. Coefficient of Determination: R^2

$$0 \le R^2 = \frac{\|\mathbf{X}\hat{\beta} - \bar{\mathbf{Y}}\mathbf{1}\|^2}{\|\mathbf{Y} - \bar{\mathbf{Y}}\mathbf{1}\|^2} = 1 - \frac{\|\mathbf{Y} - \mathbf{X}\hat{\beta}\|^2}{\|\mathbf{Y} - \bar{\mathbf{Y}}\mathbf{1}\|^2} \le 1$$

proportion of variation of Y explained by the model.

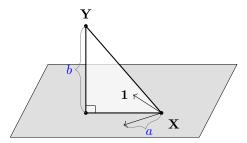


Figure 1.1. Orthogonal projection of \mathbf{Y} on plan generated by the base described by \mathbf{X} . a corresponds to $\|\mathbf{X}\hat{\beta} - \bar{\mathbf{Y}}\|^2$ and b corresponds to $\|\mathbf{Y} - \hat{\beta}\mathbf{X}\|^2$

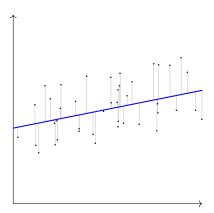


Figure 1.2. Ordinary least squares and regression line with simulated data.

Elements of Linear Algebra

Remark 1: vector

Let u a vector, we will use interchangeably the following notations: u and \vec{u}

Let
$$u = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}$$
 and $v = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$

Definition 3: Scalar Product (Dot Product)

$$\langle u, v \rangle = \begin{pmatrix} u_1, \dots, u_v \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$

= $u_1 v_1 + u_2 v_2 + \dots + u_n v_n$

We may use $\langle u, v \rangle$ or $u \cdot v$ notations.

Dot product properties

- $\langle u, v \rangle = \langle v, u \rangle$
- $\langle (u+v), w \rangle = \langle u, w \rangle + \langle v, w \rangle$
- $\langle u, v \rangle$
- $\langle \vec{u}, \vec{v} \rangle = ||\vec{u}|| \times ||\vec{v}|| \times \widehat{\cos(\vec{u}, \vec{v})}$

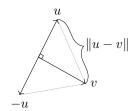


Figure 2.1. Scalar product of two orthogonal vectors.

Definition 4: Norm

Length of the vector.

$$||u|| = \sqrt{\langle u, v \rangle}$$

||u,v|| > 0

Definition 5: Distance

dist(u, v) = ||u - v||

Definition 6: Orthogonality

Remark 2

$$(dist(u,v))^2 = ||u-v||^2,$$

and

$$\langle v - u, v - u \rangle$$

$$\begin{split} \langle v-u,v-u\rangle &= \langle v,v\rangle + \langle u,u\rangle - 2\langle u,v\rangle \\ &= \|v\|^2 + \|u\|^2 \\ &= -2\langle u,v\rangle \end{split}$$

$$||u - v||^2 = ||u||^2 + ||v||^2 - 2\langle u, v \rangle$$
$$||u + v||^2 = ||u||^2 + ||v||^2 + 2\langle u, v \rangle$$

Proposition 1: Scalar product of orthogonal vectors

 $u \perp v \Leftrightarrow \langle u, v \rangle = 0$

Indeed. $||u-v||^2 = ||u+v||^2$, as illustrated in Figure 2.1.

$$\Leftrightarrow$$
 $-2\langle u, v \rangle = 2\langle u, v \rangle$

$$\Leftrightarrow 4\langle u, v \rangle = 0$$

$$\Leftrightarrow \langle u, v \rangle = 0$$



Theorem 1

Pythagorean theorem If $u \perp v$, then $||u+v||^2 = ||u||^2 + ||v||^2$.



Definition 7: Orthogonal Projection

Let $y = \begin{pmatrix} y_1 \\ y_n \end{pmatrix} \in \mathbb{R}^n$ and w a subspace of \mathbb{R}^n \mathcal{Y} can be written as the orthogonal projection of y on w:

$$\mathcal{Y} = proj^{w}(y) + z,$$

where

$$\begin{cases} z \in w^{\perp} \\ proj^{w}(y) \in w \end{cases}$$

There is only one vector \mathcal{Y} that ?

The scalar product between z and (?) is zero.

Property 1. $proj^{w}(y)$ is the closest vector to y that belongs to w.



Definition 8: Matrix

A matrix is an application, that is, a function that transform a thing into another, it is a linear function.



Example 2: Matrix application

Let A be a matrix:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

and

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Then,

$$Ax = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$
$$= \begin{pmatrix} ax_1 + bx_2 \\ cx_1 + dx_2 \end{pmatrix}$$

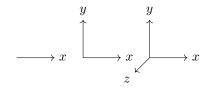


Figure 2.2. Coordinate systems

Similarly,

$$\begin{pmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \left(ax_1 + bx_2 + cx_3 \dots \right)$$

The number of columns has to be the same as the dimension of the vector to which the matrix is applied.

Definition 9: Tranpose of a Matrix

Let
$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$
, then $A^{\mathrm{T}} = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$