Statistical Models 2021

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CIMAT

Multivariate Normal Distribution

Let be

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{x} \end{pmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_y \\ \mu_x \end{bmatrix}, \begin{bmatrix} \Sigma_{yy} & \Sigma_{yx} \\ \Sigma_{xy} & \Sigma_{xx} \end{bmatrix} \right)$$

Then

$$\mathbf{y}|\mathbf{x} \sim \mathcal{N}\left(\mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(\mathbf{x} - \mu_x),\, \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy} \right)$$

Proof:

Consider the matrix

$$A = \begin{bmatrix} I & -\Sigma_{yx}\Sigma_{xx}^{-1} \\ \mathbf{0} & I \end{bmatrix}$$

and let be $\mu = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}$ and $\Sigma = \begin{bmatrix} \Sigma_{yy} & \Sigma_{yx} \\ \Sigma_{xy} & \Sigma_{xx} \end{bmatrix}$

Thus, $A\begin{pmatrix}\mathbf{y}\\ \mathbf{x}\end{pmatrix} \sim \mathcal{N}\left(A\mu,\ A\Sigma A^T\right)$. Now, let us compute this expressions

$$A\begin{pmatrix}\mathbf{y}\\ \mathbf{x}\end{pmatrix} = \begin{pmatrix}\mathbf{y} - \Sigma_{yx}\Sigma_{xx}^{-1}\mathbf{x}\\ \mathbf{x}\end{pmatrix} \equiv \begin{pmatrix}\mathbf{u}\\ \mathbf{x}\end{pmatrix}$$

$$A\mu = \begin{pmatrix}\mu_y - \Sigma_{yx}\Sigma_{xx}^{-1}\mu_x\\ \mu_x\end{pmatrix}$$

$$\begin{aligned}
A\Sigma A^T &= \begin{pmatrix}\Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy} & \Sigma_{yx} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xx}\\ \Sigma_{xy} & \Sigma_{xx}\end{pmatrix} A^T\\
&= \begin{pmatrix}\Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy} & \mathbf{0}\\ \Sigma_{xy} & \Sigma_{xx}\end{pmatrix}\begin{pmatrix}I & \mathbf{0}\\ -\Sigma_{xx}^{-1}\Sigma_{xy} & I\end{pmatrix}\\
&= \begin{pmatrix}\Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy} & \mathbf{0}\\ \mathbf{0} & \Sigma_{xx}\end{pmatrix}
\end{aligned}$$

Because

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{x} \end{pmatrix}$$

is a (multivariate) normal variable and $\text{Cov}(\mathbf{u}, \mathbf{x}) = 0$, it implies that $\mathbf{u}$ and $\mathbf{x}$ are independent, and hence $\mathbf{u}|\mathbf{x}$ has the same distribution than $\mathbf{u}$, that is

$$\mathbf{u}|\mathbf{x} \sim \mathcal{N}\left(\mu_y - \Sigma_{yx}\Sigma_{xx}^{-1}\mu_x,\, \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}\right)$$

That is,

$$\mathbf{y} - \Sigma_{yx}\Sigma_{xx}^{-1}\mathbf{x}|\mathbf{x} \sim \mathcal{N}\left(\mu_y - \Sigma_{yx}\Sigma_{xx}^{-1}\mu_x,\, \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}\right)$$

And from here, we conclude

$$\mathbf{y}|\mathbf{x} \sim \mathcal{N}\left(\mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(\mathbf{x} - \mu_x),\, \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}\right)$$

$\square$

Define

$$\begin{aligned}\mu_{y|x} &= \mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(\mathbf{x} - \mu_x) \\ &= \left[\mu_y - \Sigma_{yx}\Sigma_{xx}^{-1}\mu_x\right] + \left[\Sigma_{yx}\Sigma_{xx}^{-1}\right]\mathbf{x} \\ &\equiv \beta_0 + \beta_1\mathbf{x}\end{aligned}$$

and

$$\Sigma_{y|x} = \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}$$

Remember that

$$\Sigma_{yy} = \mathbb{E}_{\mathbf{y}}\left[(\mathbf{y} - \mu_y)(\mathbf{y} - \mu_y)^T\right]^2 \quad (\text{resp. } \Sigma_{xx})$$

and

$$\Sigma_{yx} = \mathbb{E}_{\mathbf{y},\mathbf{x}}\left[(\mathbf{y} - \mu_y)(\mathbf{x} - \mu_x)^T\right] \quad (\text{similarly } \Sigma_{xy} = \Sigma_{yx}^T)$$

Assume for now that $\mathbf{x} \equiv x \in \mathbb{R}$ and $\mathbf{y} \equiv y \in \mathbb{R}$, and that we count with a sample $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$ from independent and identically distributed random variables with the same distribution than the generic vector (x, y).
Thus (intuitively) good estimators of the previous quantities would be given by

- $\widehat{\Sigma}_{yy} \equiv S_{yy} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$ (resp. S_{xx})
- $\widehat{\Sigma}_{yx} \equiv S_{yx} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})(x_i - \bar{x}) = S_{xy}$
- $\hat{\mu}_{y|x} \equiv \hat{y}|x = \hat{\beta}_0 + \hat{\beta}_1 x$ where

$$\hat{\beta}_0 = \bar{y} - S_{yx}S_{xx}^{-1}\bar{x}$$

$$\hat{\beta}_1 = S_{yx}S_{xx}^{-1}$$

- $\widehat{\Sigma}_{y|x} \equiv \hat{\sigma}^2 = S_{yy} - S_{yx}S_{xx}^{-1}S_{xy}$

Let be $\hat{y}_i = \hat{y}_i | x_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$, $i = 1, \ldots, n$, we define the Sum of Squared Estimate Errors (SSE) (Suma de Cuadrados del Error (SCE), in Spanish) also known as Sum of Squared Residuals (SSR) or Residual Sum of Squares (RSS)

Definition 1 Sum of Squared Estimate Errors (SSE)

$$ESS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Remember that $\hat{y}_i = \bar{y} + S_{yx} S_{xx}^{-1} (x_i - \bar{x})$, thus applying simple algebra we get

$$
\begin{aligned}
SSE &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\
&= \sum_{i=1}^{n}(y_i - \bar{y})^2 + S_{yx}S_{xx}^{-1}\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)S_{xx}^{-1}S_{xy} \\
&\quad - 2\sum_{i=1}^{n}(y_i - \bar{y})S_{yx}S_{xx}^{-1}(x_i - \bar{x}) \\
\frac{1}{n}SSE &= S_{yy} + S_{yx}\cancel{S_{xx}^{-1}}\cancel{S_{xx}}S_{xx}^{-1}S_{xy} - 2S_{yx}S_{xx}^{-1}S_{xy} \\
&= S_{yy} - S_{yx}S_{xx}^{-1}S_{xy}
\end{aligned}
$$

Linear Regression

Mathematical modeling refers to the construction of mathematical expressions that describes the behavior of a variable of interest Y. Frequently we want to add to the model some variables (features) X, which give information about the variable of interest Y denoted as response.

In regression analysis one considers (X, Y) as random vector, where X is $\mathbb{R}^p$-valued ($X \in \mathcal{X} \subseteq \mathbb{R}^p$) and Y is $\mathbb{R}$-valued ($Y \in \mathcal{Y} \subset \mathbb{R}$). We are interested on how the variable Y depends on the value of the observation vector X. This means that we want to find a function $f : \mathcal{X} \to \mathcal{Y}$, such that $f(X)$ is a good approximation of Y, that is, $f(X)$ should be close to Y in some sense, which is equivalent to making $|f(X) - Y|$ "small". Since X and Y are random vectors, $|f(X) - Y|$ is random as well, therefore it is not clear what "small $|f(X) - Y|$" means.

We can resolve this problem by introducing the so-called L_2 risk or mean squared error of f,

$$\mathbb{E}_{X,Y}\left[f(X) - Y\right]^2,$$

and requiring it to be as small as possible. So we are interested in a (measurable) function $m : \mathcal{X} \to \mathcal{Y}$ such that

$$m = \underset{f:\mathcal{X}\to\mathcal{Y}}{\arg\min}\, \mathbb{E}_{X,Y}\left[f(X) - Y\right]^2$$

Such function that minimizes the mean squared error is given by the regression function

$$m(X) = \mathbb{E}[Y|X]$$

Proof:
For any arbitrary function $f : \mathcal{X} \to \mathcal{Y}$,

$$\begin{aligned}
\mathbb{E}_{X,Y}\left[f(X) - Y\right]^2 &= \mathbb{E}_{X,Y}\left[f(X) - m(X) + m(X) - Y\right]^2 \\
&= \mathbb{E}_{X,Y}\left[f(X) - m(X)\right]^2 + \mathbb{E}_{X,Y}\left[m(X) - Y\right]^2,
\end{aligned}$$

where we have used

$$\begin{aligned}
&\mathbb{E}_{X,Y}\left[(f(X) - m(X))(m(X) - Y)\right] \\
&= \mathbb{E}_X\left\{\mathbb{E}_{Y|X}\left[(f(X) - m(X))(m(X) - Y)\right]\right\} \\
&= \mathbb{E}_X\left\{(f(X) - m(X))\mathbb{E}_{Y|X}\left[(m(X) - Y)\right]\right\} \\
&= \mathbb{E}_X\left\{(f(X) - m(X))(m(X) - m(X))\right\} \\
&= 0
\end{aligned}$$

Thus,

$$
\begin{aligned}
&\arg\min_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{X,Y}\left[f(X) - Y\right]^2 \\
&= \arg\min_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{X,Y}\left[f(X) - m(X)\right]^2 + \mathbb{E}_{X,Y}\left[m(X) - Y\right]^2 \\
&= \arg\min_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{X}\left[f(X) - m(X)\right]^2
\end{aligned}
$$

Note that $\mathbb{E}_X\left[f(X) - m(X)\right]^2$, called the L_2 error of f is nonnegative and is zero if $f(X) = m(X)$. Therefore

$$
m = \arg\min_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{X,Y}\left[f(X) - Y\right]^2
$$

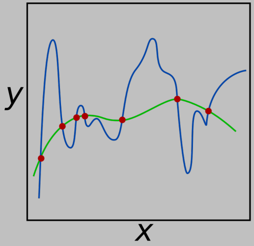
$\square$

For practical problems, the distribution of (X, Y) is unknown and hence, the regression function is unknown as well. However, in our framework, we have access to a training set $\mathcal{D}_n = (X_i, Y_i)_{i=1,\ldots,n}$ where the collected data has the same distribution than (X, Y) and are considered independent. The goal is to use the data $\mathcal{D}_n$ to construct a learning model, also called learner or predictor, $m_n : \mathcal{X} \to \mathcal{Y}$ which estimates the function m, and enables us to predict the outcome for new unseen objects.

Thus, instead of minimizing the L_2 risk we minimize the empirical L_2 risk

$$\mathbb{E}_{\mathcal{D}_n}[f(X) - Y]^2 = \frac{1}{n}\sum_{i=1}^{n}[f(X_i) - Y_i]^2$$

Note that minimizing the above expression over all the functions $f : \mathcal{X} \to \mathcal{Y}$ is not well-define, since every function which takes the value Y_i for every X_i would have zero empirical risk.



[1]

[1] picture taken from Wikipedia: https://en.wikipedia.org/wiki/Regularization_(mathematics)

We can resolve this problem restricting the search of the function that minimizes the empirical risk into a pre-defined set of functions $\mathcal{F}$. Moreover, the parametric estimation uses a model belonging to a set of functions $\mathcal{F}_\Theta$ determined by a finite number of parameters Θ, then the estimation is made through the inference of this set of parameters that minimize the empirical risk,

$$m_n = m_n(\cdot, \hat{\theta}) = \underset{f_\theta \in \mathcal{F}_\Theta}{\arg\min}\, \mathbb{E}_{\mathcal{D}_n}[f_\theta(X) - Y]^2,$$

where

$$\hat{\theta} = \underset{\theta \in \Theta}{\arg\min}\, \mathbb{E}_{\mathcal{D}_n}[f_\theta(X) - Y]^2$$

For example let be $\mathcal{F}_\Theta = \{f : \mathcal{X} \to \mathcal{Y} : f(X) = X^T\beta, \beta \in \mathbb{R}^p\}$ $(\Theta = \{\beta : \beta \in \mathbb{R}^p\})$,

$$m_n(X) = X^T\hat{\beta} = \underset{f_\theta \in \mathcal{F}_\Theta}{\arg\min}\, \mathbb{E}_{\mathcal{D}_n}[f_\theta(X) - Y]^2$$

where

$$\begin{aligned}\hat{\beta} &= \underset{\beta \in \mathbb{R}^p}{\arg\min}\, \mathbb{E}_{\mathcal{D}_n}[X^T\beta - Y]^2 \\ &= \underset{\beta \in \mathbb{R}^p}{\arg\min} \sum_{i=1}^{n} [X_i^T\beta - Y_i]^2\end{aligned}$$

This is known as Ordinary Leas Squares (OLS).

Let be $\mathbf{X} = \begin{bmatrix} X_1^T \\ \vdots \\ X_n^T \end{bmatrix}$ and $\mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix}$, $\mathbf{X}$ is known as the design matrix while $\mathbf{Y}$ is known as the response vector. Then

$$\sum_{i=1}^{n} [X_i^T \beta - Y_i]^2$$

can be written as

$$\begin{aligned} \sum_{i=1}^{n} [X_i^T \beta - Y_i]^2 &= [\mathbf{X}\beta - \mathbf{Y}]^T [\mathbf{X}\beta - \mathbf{Y}] \\ &= [\beta^T \mathbf{X}^T - \mathbf{Y}^T][\mathbf{X}\beta - \mathbf{Y}] \\ &= \beta^T \mathbf{X}^T \mathbf{X}\beta - 2\beta^T \mathbf{X}^T \mathbf{Y} + \mathbf{Y}^T \mathbf{Y}, \end{aligned}$$

$\hat{\beta}$ can be obtained from the right-hand side of the above expression.

$\hat{\beta}$ satisfies

$$\frac{\partial}{\partial\beta}(\beta^T\mathbf{X}^T\mathbf{X}\beta - 2\beta^T\mathbf{X}^T\mathbf{Y} + \mathbf{Y}^T\mathbf{Y})\Big|_{\hat{\beta}} = 0$$

That is,

$$\begin{aligned} 2\mathbf{X}^T\mathbf{X}\hat{\beta} - 2\mathbf{X}^T\mathbf{Y} &= 0 \\ \Leftrightarrow \mathbf{X}^T(\mathbf{Y} - \mathbf{X}\hat{\beta}) &= 0 \qquad (1) \end{aligned}$$

Equation (1) is known as the **normal equations**. It is easy to see that $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}\mathbf{Y}$.

Hence, under this model, the best prediction $\widehat{\mathbf{Y}}$ for the vector of response $\mathbf{Y}$ is given by

$$\begin{aligned}\widehat{\mathbf{Y}} = \begin{bmatrix}\widehat{Y}_1\\ \vdots \\ \widehat{Y}_n\end{bmatrix} &= \begin{bmatrix}X_1^T\\ \vdots \\ X_n^T\end{bmatrix}\hat{\beta}\\ &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}\end{aligned}$$

Let be $\mathbf{P} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$, so $\widehat{\mathbf{Y}} = \mathbf{P}\mathbf{Y}$.
We will see that $\widehat{\mathbf{Y}}$ is the orthogonal projection of $\mathbf{Y}$ over the span of the the columns of $\mathbf{X}$ (What does this mean?).

Projections

Let $\mathbf{X} = \left[\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(p)}\right]$ be an $n \times p$ matrix, let $W = \mathrm{Col}(\mathbf{X})$, and let $\mathbf{Y}$ be a vector in $\mathbb{R}^n$.
Let $\mathbf{Y} = \mathbf{Y}_W + \mathbf{Y}_{W^\perp}$ be the orthogonal decomposition with respect to W. By definition $\mathbf{Y}_W$ lies in $W = \mathrm{Col}(\mathbf{X})$ so there is a vector $\hat{\beta} \in \mathbb{R}^p$ with $\mathbf{Y}_W = \mathbf{X}\beta$, that is

$$\begin{aligned}
\mathbf{Y}_W &= \mathbf{X}\hat{\beta} \\
&= \left[\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(p)}\right] \begin{bmatrix} \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_p \end{bmatrix} \\
&= \hat{\beta}_1 \mathbf{X}^{(1)} + \cdots + \hat{\beta}_p \mathbf{X}^{(p)}
\end{aligned}$$

Choose any such vector $\hat{\beta}$. We know that $\mathbf{Y} - \mathbf{Y}_W = \mathbf{Y} - \mathbf{X}\hat{\beta}$ lies in $W^{\perp}$, which is equal to $\mathrm{Null}(\mathbf{X}^T)$. We thus have

$$0 = \mathbf{X}^T(\mathbf{Y} - \mathbf{X}\hat{\beta}) = \mathbf{X}^T\mathbf{Y} - \mathbf{X}^T\mathbf{X}\hat{\beta}$$

and so

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

Hence,

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

Remember that $\mathbf{Y}_W = \mathbf{X}\hat{\beta}$, so it can be written as

$$\begin{aligned}\mathbf{Y}_W &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\ &= \mathbf{P}\mathbf{Y}\end{aligned}$$

where $\mathbf{P} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$.
Thus, $\mathbf{P}$ is a projection matrix over the columns of $\mathbf{X}$. Actually is the orthogonal projection onto $\mathrm{Col}(\mathbf{X})$.

Properties of a Projection Matrix

- If $\mathbf{P}$ is a projection matrix in a space W, then $\mathbf{P}^2 = \mathbf{P}$. Remember that a vector that has been projected onto W belongs to that space, thus projecting again over W would led the same result.
- If $\mathbf{P} = \mathbf{P}^T$, then $\mathbf{P}$ is the creates orthogonal projections onto W.

Suppose that $\mathbf{P}$ satisfies both conditions, and consider its SVD decomposition, so

$$\mathbf{P} = USV^T$$

where U and V are orthogonal matrices. (An orthogonal matrix satisfies: $Q^TQ = QQ^T = I$).

Actually, U and V are rotation or reflection matrices. So, we might think as if the projection is "computed" by S.
Because $\mathbf{P}^2 = \mathbf{P}$,

$$USV^T USV^T = USV^T$$

which implies $SV^T US = S$.
Using the fact that $\mathbf{P} = \mathbf{P}^T$, we get that $USV^T = VSU^T$. So $U = V$.
Therefore, it is satisfied

$$US^2U^T = USU^T$$

Since

$$S = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_p \end{bmatrix}$$

Then $\lambda_i \in \{0, 1\}$

Those places where $\lambda_i = 1$ represent the coordinates (in the rotated space) where the projection is perform, the basis of W. On the other hand, the places where $\lambda_i = 0$ would lead to a basis for $W^\perp$.

Example 1

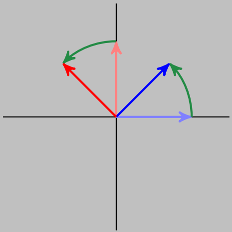
Consider the matrix

$$\mathbf{P} = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}$$

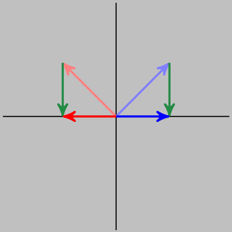
which can be written as

$$\mathbf{P} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

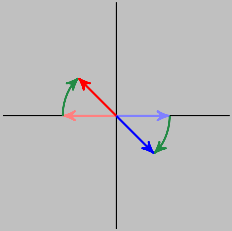
$$\mathbf{P} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$



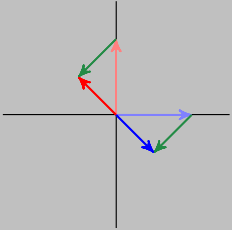
$$\begin{aligned} \mathbf{P} &= \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \\ &= \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 0 \end{bmatrix} \end{aligned}$$



$$\mathbf{P} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}$$



$$\mathbf{P} = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}$$



Example 2

Let $\mathbf{X} = [\mathbf{X}^{(1)}] = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$

It can be shown that

$$\mathbf{P} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}$$

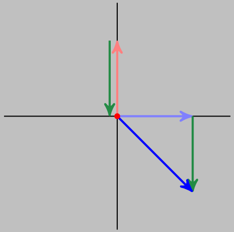
so $\mathbf{P}$ is the orthogonal projection onto Span $\left(\mathbf{X}^{(1)}\right)$

Now, consider the matrix

$$\mathbf{P}' = \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}$$

note that $\mathbf{P}'^2 = \mathbf{P}'$, hence $\mathbf{P}'$ is a projection matrix.

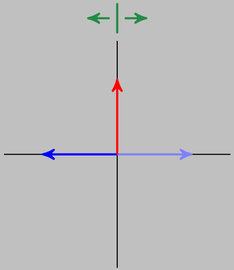
$$\mathbf{P}' = \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}$$



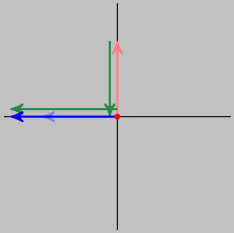
$\mathbf{P}'$ is an oblique projection onto Span $\left(\mathbf{X}^{(1)}\right)$.
The SVD decomposition of $\mathbf{P}'$ is

$$\mathbf{P}' = \underbrace{\begin{bmatrix} -1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}}_{U'} \underbrace{\begin{bmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{bmatrix}}_{S'} \underbrace{\begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix}}_{V'^T}$$

$$\mathbf{P}' = \begin{bmatrix} -1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix}$$

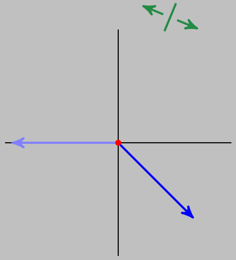


$$\mathbf{P}' = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix}$$
$$= \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} -\sqrt{2} & 0 \\ 0 & 0 \end{bmatrix}$$



$$\mathbf{P}' = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} -\sqrt{2} & 0 \\ 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}$$



Let be $\mathbf{Z} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and

$$\mathbf{P_Z} = \mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

Moreover, let $\mathbf{B} = \mathbf{P_Z X}$ be the orthogonal projection of $\mathbf{X}$ onto $\mathrm{Col}(\mathbf{Z})$,

$$\mathbf{B} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$$

Simple calculations show $\mathbf{P'} = \mathbf{X}(\mathbf{B}^T\mathbf{X})^{-1}\mathbf{B}^T$.
Define $\mathbf{Y}_{\mathrm{IV}} = (\mathbf{X}(\mathbf{B}^T\mathbf{X})^{-1}\mathbf{B}^T)\mathbf{Y}$, $\mathbf{Y}_{\mathrm{IV}}$ is an oblique projection over $\mathrm{Col}(\mathbf{X})$.
This method is called **Two-Stage Least Squares (2SLS)**.
In the first stage we get the orthogonal projection of $\mathbf{X}$ onto $\mathrm{Col}(\mathbf{Z})$, where $\mathbf{Z}$ is called **instrumental variables**.

Linear Regression (2)

Consider the model

$$Y_i = X_i^T \beta + \varepsilon_i,\ i = 1, \ldots, n$$

where $\mathbb{E}[\varepsilon_i | X_i] = 0, \quad \forall i = 1, \ldots, n.$

So $\mathbb{E}[Y_i | X_i] = X_i^T \beta$, and that $\varepsilon_i = Y_i - X_i^T \beta$. $\varepsilon_i,\ i = 1, \ldots, n$ are called the **errors of the model**.

Denote by $\boldsymbol{\varepsilon}$ the vector with these errors,

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

Consider $\hat{\beta} = \mathbf{P}\mathbf{Y}$, where $\mathbf{P} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$

Let be $\widehat{\mathbf{Y}} = \mathbf{X}\hat{\beta}$ ($\widehat{Y}_i = X_i^T\hat{\beta}$). Then $Y_i - \widehat{Y}_i$, $i = 1\ldots, n$, called the **residuals of the model**, estimate the errors ε_i, $i = 1, \ldots, n$ and $\mathbf{Y} - \widehat{\mathbf{Y}}$ estimates $\boldsymbol{\varepsilon}$.

Denote by $\mathbf{e} = \mathbf{Y} - \widehat{\mathbf{Y}}$ the vector of residuals, note that $\mathbf{e} = (\mathbf{I} - \mathbf{P})\mathbf{Y}$.

Moreover, it is easy to show that $\mathbf{I} - \mathbf{P}$ is the projection matrix onto $\mathrm{Col}(\mathbf{X})^{\perp}$, hence $\mathbf{X}^T\mathbf{e} = \mathbf{0}$

Writing $\mathbf{X} = \left[\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(p)}\right]$,

$$\mathbf{X}^T\mathbf{e} = \begin{bmatrix} \mathbf{X}^{(1)T}\mathbf{e} \\ \vdots \\ \mathbf{X}^{(p)T}\mathbf{e} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n X_i^{(1)} e_i \\ \vdots \\ \sum_{i=1}^n X_i^{(p)} e_i \end{bmatrix}$$

We can conclude that $\sum_{i=1}^n X_i^{(h)} e_i = 0$, for all $h \in \{1, \ldots, p\}$.
For example, if

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

We have proved that $\sum_{i=1}^n e_i = 0$ and $\sum_{i=1}^n x_i e_i = 0$

Distributional Properties

Let be $y \sim \mathcal{N}(\mu, \sigma^2 \mathbf{I})$, then

1. $Ay \perp By \iff AB^T = 0$.
2. $Ay \perp y^T C y \iff AC = 0$, where C is non-negative definite.
3. $y^T C y \perp y^T D y \iff CD = 0$, where C and D are non-negative definite.

Let be $y \sim \mathcal{N}(\mu, \Sigma)$, then $y^T A y \sim \chi^2_{k,\lambda}$ if and only if $A\Sigma$ is symmetric and idempotent of range k, where $\lambda = \frac{1}{2}\mu^T A \mu$.

Assume $\mathbf{Y}|\mathbf{X} \sim \mathcal{N}(\mathbf{X}\beta, \sigma^2\mathbf{I})$, which is equivalent to the assumption $\varepsilon_i|X_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2)$.
Consider the least squares estimate $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$, then

- $$\hat{\beta}|\mathbf{X} \sim \mathcal{N}(\beta, \sigma^2(\mathbf{X}^T\mathbf{X})^{-1})$$

Remember that $SSE = (\mathbf{Y} - \widehat{\mathbf{Y}})^T(\mathbf{Y} - \widehat{\mathbf{Y}}) = (\mathbf{Y} - \mathbf{PY})^T(\mathbf{Y} - \mathbf{PY}) = \mathbf{Y}^T(\mathbf{I} - \mathbf{P})\mathbf{Y}$, then

- $$\frac{SSE}{\sigma^2} = \mathbf{Y}^T \frac{\mathbf{I} - \mathbf{P}}{\sigma^2} \mathbf{Y}$$

  and

  $$\frac{SSE}{\sigma^2} | \mathbf{X} \sim \chi^2_{n-p}$$

Denote by $\hat{\sigma}^2$ the unbiased estimate of σ, $\hat{\sigma}^2 = \frac{SSE}{n-p}$, then

- $$\hat{\beta} \perp \hat{\sigma}^2 | \mathbf{X}$$

To see this, remember that $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ and $\hat{\sigma}^2 = \frac{1}{n-p}\mathbf{Y}^T(\mathbf{I}-\mathbf{P})\mathbf{Y}$. Hence $\hat{\beta}$ and $\hat{\sigma}^2$ are independent if and only if

$$\frac{1}{n-p}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{I}-\mathbf{P}) = \mathbf{0}$$

As a consequence of the previous results, we have that

- $$\frac{(n-p)\hat{\sigma}^2}{\sigma^2}|\mathbf{X} \sim \chi^2_{n-p}$$
- $$\frac{a^T\hat{\beta} - a^T\beta}{\sqrt{\sigma^2 a^T(\mathbf{X}^T\mathbf{X})^{-1}a}}|\mathbf{X} \sim \mathcal{N}_1(0,1), \quad \forall a \in \mathbb{R}^p, a \neq 0$$
- $$\frac{a^T\hat{\beta} - a^T\beta}{\sqrt{\hat{\sigma}^2 a^T(\mathbf{X}^T\mathbf{X})^{-1}a}}|\mathbf{X} \sim t_{n-p}, \quad \forall a \in \mathbb{R}^p, a \neq 0$$

- $$(\hat{\beta} - \beta)^T \frac{\mathbf{X}^T\mathbf{X}}{\sigma^2} (\hat{\beta} - \beta) | \mathbf{X} \sim \chi_p^2$$
- $$(\hat{\beta} - \beta)^T \frac{\mathbf{X}^T\mathbf{X}}{p\hat{\sigma}^2} (\hat{\beta} - \beta) | \mathbf{X} \sim F_{n-p}^p$$

Confidence Intervals/Region

- A $(1-\alpha) \times 100\%$ confidence interval for $a^T\beta$ is given by

$$a^T\hat{\beta} \pm t_{n-p,\alpha/2}\sqrt{\hat{\sigma}^2 a^T(\mathbf{X}^T\mathbf{X})^{-1}a}$$

- A $(1-\alpha) \times 100\%$ confidence interval for β_j is given by

$$\hat{\beta}_j \pm t_{n-p,\alpha/2}\sqrt{\hat{\sigma}^2(\mathbf{X}^T\mathbf{X})^{-1}_{j,j}}$$

  where $\beta = [\beta_1, \ldots, \beta_p]^T$
- A $(1-\alpha) \times 100\%$ confidence region for β is given by

$$\left\{\beta : (\hat{\beta}-\beta)^T \frac{\mathbf{X}^T\mathbf{X}}{p\hat{\sigma}^2}(\hat{\beta}-\beta)|\mathbf{X} \leq F^p_{n-p,1-\alpha}\right\}$$

Prediction Interval

Remember that $Y = X^T\beta + \varepsilon$,

$$Y|X \sim \mathcal{N}(X^T\beta, \sigma^2)$$

and $\widehat{Y} = X^T\hat{\beta}$,

$$\widehat{Y}|(X, \mathbf{X}) \sim \mathcal{N}(X^T\beta, \sigma^2 X^T(\mathbf{X}^T\mathbf{X})^{-1}X)$$

Because $Y \perp \hat{Y}|\mathbf{X}$, then

$$Y - \widehat{Y}|(X, \mathbf{X}) \sim \mathcal{N}(0, \sigma^2(1 + X^T(\mathbf{X}^T\mathbf{X})^{-1}X))$$

Therefore,

$$\frac{Y-\widehat{Y}}{\sqrt{\hat{\sigma}^2(1+X^T(\mathbf{X}^T\mathbf{X})^{-1}X)}}|(X,\mathbf{X}) \sim t_{n-p}$$

- A $(1-\alpha)\times 100\%$ prediction interval for Y is given by

$$X^T\hat{\beta} \pm t_{n-p,\alpha/2}\sqrt{\hat{\sigma}^2(1+X^T(\mathbf{X}^T\mathbf{X})^{-1}X)}$$