Linear Regression 2
DS351

Linear algebra revisited 1

The identity matrix

$$I_n = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}$$

An inverse of a $n \times n$ **square matrix** X is a matrix X^{-1} such that

$$XX^{-1} = X^{-1}X = I_n.$$

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Linear algebra revisited 2

Two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ are perpendicular if

$$\boldsymbol{u} \cdot \boldsymbol{v} = \boldsymbol{u}^T \boldsymbol{v} = 0$$

Linear Regression

- Quantitative response Y.
- Predictor variable $X_1, X_2, \ldots, X_n$.

Goal: Study a linear relationship between X_i's and Y:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_p X_p + \epsilon.$$

Again, ϵ is a random variable with zero mean and unknown variance.

Example: We study the effects of TV, radio and newspaper advertising budgets on the sales of a product.

$$sales = \beta_0 + \beta_1 \times TV + \beta_2 \times radio + \beta_3 \times newspaper + \epsilon.$$

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Data: $(\boldsymbol{x}_i, y_i)$ where $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$.
As in the simple case, we find the estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ which give the prediction

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \ldots + \hat{\beta}_p x_{ip},$$

and we want to minimize the RSS

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \ldots - \hat{\beta}_p x_{ip})^2 \end{aligned}$$

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Equations in a matrix form

Let

$$\widehat{\boldsymbol{Y}} = (\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n)^T$$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \ldots & x_{1p} \\ 1 & x_{21} & x_{22} & \ldots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \ldots & x_{np} \end{pmatrix}$$

$$\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_p)^T.$$

. Then the linear equations can be written as

$$\widehat{\boldsymbol{Y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}}.$$

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$$\widehat{\boldsymbol{Y}} = \mathbf{1}\hat{\beta}_0 + \boldsymbol{X}_1\hat{\beta}_1 + \boldsymbol{X}_2\hat{\beta}_2 + \ldots + \boldsymbol{X}_p\hat{\beta}_p$$

Find $\hat{\beta}$ such that $\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}$ is perpendicular to $\boldsymbol{X}_0, \boldsymbol{X}_1, \ldots, \boldsymbol{X}_p$.
In other words,

$$\boldsymbol{X}_i \cdot \left(\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}\right) = \boldsymbol{X}_i^T \left(\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}\right) = 0 \qquad i = 0, 1, \ldots, p.$$

$$\begin{pmatrix} \longleftarrow & \boldsymbol{X}_0 & \longrightarrow \\ \longleftarrow & \boldsymbol{X}_1 & \longrightarrow \\ & \vdots & \\ \longleftarrow & \boldsymbol{X}_p & \longrightarrow \end{pmatrix} \left(\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}\right) = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

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OLS estimator $\hat{\boldsymbol{\beta}}$

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

Variance-covariance of the estimators

$$\begin{aligned}\mathrm{Cov}\hat{\boldsymbol{\beta}} &= \mathrm{Var}((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}) \\ &= \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}\end{aligned}$$

Since σ^2 is unknown, we instead use its estimator

$$\mathrm{RSE} = \sqrt{\frac{RSS}{n-p-1}}.$$

What we will use instead of $\mathrm{Cov}\hat{\boldsymbol{\beta}}$ is

$$C = \mathrm{RSE}^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}$$

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Example

In the following regression:

$$\widehat{sales} = \hat{\beta}_0 + \hat{\beta}_1 \times TV + \hat{\beta}_2 \times radio + \hat{\beta}_3 \times newspaper,$$

We have $(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3) = (2.939, 0.046, 0.189, -0.001)$

$\mathrm{RSE} = \sqrt{\mathrm{RSS}/(n-3-1)} = 1.69$ and

$$C = \begin{pmatrix} 9.7 \times 10^{-2} & -2.7 \times 10^{-4} & -1.1 \times 10^{-3} & -6.0 \times 10^{-4} \\ -2.7 \times 10^{-4} & 1.9 \times 10^{-6} & -4.5 \times 10^{-7} & -3.3 \times 10^{-7} \\ -1.1 \times 10^{-3} & -4.5 \times 10^{-7} & 7.4 \times 10^{-5} & -1.8 \times 10^{-5} \\ -5.9 \times 10^{-4} & -3.3 \times 10^{-7} & -1.8 \times 10^{-5} & 3.4 \times 10^{-5} \end{pmatrix}$$

$\mathrm{SE}(\hat{\beta}_3) = \sqrt{3.4 \times 10^{-5}} = 0.0059.$

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Important questions

1. Is at least one of the predictors $X_1, X_2, \ldots, X_p$ useful in predicting the response?
2. Do all predictors help explaining Y, or only a subset of them?
3. How well does model fit the data?

Relationship between the response and the predictors

We use a hypothesis test:

$$H_0 : \beta_1 = \beta_2 = \ldots = \beta_p = 0$$
$$H_a : \text{at least one of } \beta_j\text{'s is non-zero.}$$

The decision will be made after looking at the F–statistic:

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS})/p}{\mathrm{RSS}/(n-p-1)}.$$

Recall that $\mathrm{TSS} = \sum_{i=1}^{n}(y_i - \bar{y})^2$ and $\mathrm{RSS} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$.

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How should we look at $F-$ statistic?

One can show that

$$\mathbb{E}[\mathrm{RSS}/(n-p-1)] = \sigma^2$$

and provided that H_0 is true, we also have

$$\mathbb{E}[(\mathrm{TSS}-\mathrm{RSS})/p] = \sigma^2.$$

- If H_0 is true, then we expect F–statistic to be **very close to 1**.
- If H_a is true, then $\mathbb{E}[(\mathrm{TSS}-\mathrm{RSS})/p]$ and so we expect F to be **greater than 1**.

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Sales data

$$\widehat{sales} = \hat{\beta}_0 + \hat{\beta}_1 \times TV + \hat{\beta}_2 \times radio + \hat{\beta}_3 \times newspaper$$

- The F-value is 570 with its corresponding p-value $= 1.58 \times 10^{-96}$.
- We are certain that **at least** one of the advertising media must be related to the sales.

Relationship between the response and a subset of the predictors

Suppose we want to make the same test for **a subset** of q predictors:

$$H_0 : \beta_{i+1} = \beta_{i+2} = \ldots = \beta_{i+q} = 0$$
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The decision will be made after looking at the F–statistic:

$$F = \frac{(\mathrm{RSS}_{-q} - \mathrm{RSS})/q}{\mathrm{RSS}/(n-p-1)},$$

where RSS_{-q} is the residual sum of squares of the model **without those** q **predictors**.

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Relationship between the response and a single predictor

The hypothesis test is

$$H_0 : \beta_j = 0$$
$$H_a : \beta_j \neq 0$$

The decision will be made after looking at the t–statistic:

$$t = \frac{\hat{\beta}_j - 0}{\mathrm{SE}(\hat{\beta}_j)}.$$

Here, $\mathrm{SE}(\hat{\beta}_j)$ is the square root of entry (j, j) of C, which is an estimate of the covariance matrix of the coefficients.

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Example

	Coefficient	SE	t-statistic	p-value
Intercept	2.939	0.3119	9.42	< 0.0001
TV	0.046	0.0014	32.81	< 0.0001
radio	0.189	0.0086	21.89	< 0.0001
newspaper	-0.001	0.0059	-0.18	0.8599

For example, t-statistic of $\hat{\beta}_3$ (newspaper) is

$$t = \frac{-0.0001}{0.0059} = -0.18$$

Example

However, newspaper strongly affects sales in the simple linear regression.

	Coefficient	SE	t-statistic	p-value
Intercept	12.351	0.621	19.88	< 0.0001
newspaper	0.055	0.071	3.30	< 0.0001

This is because of the correlation between newspaper and radio

	TV	radio	newspaper	sales
TV	1.000	0.055	0.057	0.78
radio		1.000	0.35	0.58
newspaper			1.000	0.23
sales				1.000

Higher values of newspaper $\rightarrow$ higher values of radio, which is the one that affects the sales.

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F-statistic vs t-statistic

Why do we prefer F-statistic over t-statistic when testing $\beta_0 = \beta_1 = \ldots, \beta_p = 0$?

- Calculating F is easier than t, especially for a high p.
- For large p, even $\beta_0 = \beta_1 = \ldots, \beta_p = 0$ is true, there is a small chance that the p-value of some β_j is low enough that we reject $\beta_j = 0$. The F-statistic does not suffer from this issue since it is calculated only once.

Variable selection

- Forward selection:
  - Start with 0 variable. In each step: add a variable that results in the lowest RSS.
  - Stop when RSS barely improves by adding any of the remaining variables.
  - For example, if adding any of the remaining variables reduces the RSS by less that 0.0001, then we will stop here.
- Backward selection:
  - Start with all variables. In each step: remove a variable with the largest p-value.
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Model evaluation

- Residual standard error (RSE):

$$\text{RSE} = \sqrt{\frac{\text{RSS}}{n - p - 1}}$$

- R^2 measures the variance of Y that is explained by the model:

$$R^2 = \left[\text{Cor}(Y, \widehat{Y})\right]^2$$

Example

Predictos	RSE	R2
TV	3.26	0.612
TV + radio	1.68	0.897
TV + radio + newspaper	1.69	0.897

In both metrics, we can conclude that

- Adding `radio` helps significantly improve the model.
- There is no point in adding `newspaper` to the model.