## Linear Regression 2

229351

## Regression with Multiple Predictors

- Response Y.
- Predictors $X_{1}, X_{2}, \ldots, X_{n}$.

Goal: Study a linear relationship between $X_{i}$ 's and $Y$ :

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Y=\beta_{0}+\beta_{1} X_{1}+\beta_{2} X_{2}+\beta_{p} X_{p}+\epsilon
$$

where $\epsilon \sim N\left(0, \sigma^{2}\right), \sigma$ is unknown

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where $\epsilon \sim N\left(0, \sigma^{2}\right)$, $\sigma$ is unknown
Example: We study the effects of TV, radio and newspaper advertising budgets on the sales of a product.

$$
\text { sales }=\beta_{0}+\beta_{1} \times T V+\beta_{2} \times \text { radio }+\beta_{3} \times \text { newspaper }+\epsilon
$$

## Data

Data: $\left(\boldsymbol{x}_{1}, y_{1}\right), \ldots,\left(\boldsymbol{x}_{n}, y_{n}\right)$, where

$$
\boldsymbol{x}_{i}=\left(x_{i 1}, x_{i 2}, \ldots, x_{i p}\right) \quad i=1, \ldots, n
$$

Example:

|  | TV <br> $\left(\boldsymbol{X}_{1}\right)$ | Radio <br> $\left(\boldsymbol{X}_{2}\right)$ | Newspaper <br> $\left(\boldsymbol{X}_{3}\right)$ | Sales <br> $(\boldsymbol{Y})$ |
| ---: | ---: | ---: | ---: | ---: |
| 1 | 230.1 | 37.8 | 69.2 | 22.1 |
| 2 | 44.5 | 39.3 | 45.1 | 10.4 |
| 3 | 17.2 | 45.9 | 69.3 | 9.3 |
| 4 | 151.5 | 41.3 | 58.5 | 18.5 |
| 5 | 180.8 | 10.8 | 58.4 | 12.9 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| 200 | 232.1 | 8.6 | 8.7 | 13.4 |

As in the simple case, we find the estimates $\hat{\beta}_{0}, \hat{\beta}_{1}, \ldots, \hat{\beta}_{p}$ which give the prediction

$$
\hat{y}_{i}=\hat{\beta}_{0}+\hat{\beta}_{1} x_{i 1}+\hat{\beta}_{2} x_{i 2}+\ldots+\hat{\beta}_{p} x_{i p},
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$$

and we want to minimize the RSS

$$
\begin{aligned}
\mathrm{RSS} & =\sum_{i=1}^{n}\left(y_{i}-\hat{y}_{i}\right)^{2} \\
& =\sum_{i=1}^{n}\left(y_{i}-\hat{\beta}_{0}-\hat{\beta}_{1} x_{i 1}-\hat{\beta}_{2} x_{i 2}-\ldots-\hat{\beta}_{p} x_{i p}\right)^{2}
\end{aligned}
$$

## Equations in a matrix form

Let

$$
\begin{aligned}
\boldsymbol{Y} & =\left(y_{1}, y_{2}, \ldots, y_{n}\right)^{T} \\
\widehat{\boldsymbol{Y}} & =\left(\hat{y}_{1}, \hat{y}_{2}, \ldots, \hat{y}_{n}\right)^{T} \\
\boldsymbol{X} & =\left(\begin{array}{ccccc}
1 & x_{11} & x_{12} & \ldots & x_{1 p} \\
1 & x_{21} & x_{22} & \ldots & x_{2 p} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & x_{n 1} & x_{n 2} & \ldots & x_{n p}
\end{array}\right) \\
\hat{\boldsymbol{\beta}} & =\left(\hat{\beta}_{0}, \hat{\beta}_{1}, \hat{\beta}_{2}, \ldots, \hat{\beta}_{p}\right)^{T}
\end{aligned}
$$

Then the linear equations can be written as

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

$$
\begin{aligned}
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1 & x_{n 1} & x_{n 2} & \ldots & x_{n p}
\end{array}\right)\left(\begin{array}{c}
\hat{\beta}_{0} \\
\hat{\beta}_{1} \\
\vdots \\
\hat{\beta}_{p}
\end{array}\right) \\
\widehat{\boldsymbol{Y}} & =\mathbf{1} \hat{\beta}_{0}+\boldsymbol{X}_{1} \hat{\beta}_{1}+\boldsymbol{X}_{2} \hat{\beta}_{2}+\ldots+\boldsymbol{X}_{p} \hat{\beta}_{p}
\end{aligned}
$$

In other words, $\widehat{\boldsymbol{Y}}$ must lie in the space spanned by

$$
1, \boldsymbol{X}_{1}, \boldsymbol{X}_{2}, \ldots, \boldsymbol{X}_{p}
$$

## True Response vs Prediction


$\operatorname{Span}(\mathbb{X})$

## Finding the Best Prediction


$\operatorname{Span}(\mathbb{X})$

Find $\hat{\boldsymbol{\beta}}$ such that $\boldsymbol{Y}-\boldsymbol{X} \hat{\boldsymbol{\beta}} \perp \mathbf{1}, \boldsymbol{X}_{1}, \ldots, \boldsymbol{X}_{p}$.

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\boldsymbol{X}_{i} \cdot(\boldsymbol{Y}-\boldsymbol{X} \hat{\boldsymbol{\beta}})=0 \quad i=0,1, \ldots, p
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& \boldsymbol{X}_{i} \cdot(\boldsymbol{Y}-\boldsymbol{X} \hat{\boldsymbol{\beta}})=0 \quad i=0,1, \ldots, p \\
& \left(\begin{array}{ccll}
\longleftarrow & \boldsymbol{X}_{0} & \longrightarrow \\
\longleftarrow & \boldsymbol{X}_{1} & \longrightarrow \\
\vdots & \\
\longleftarrow & \boldsymbol{X}_{p} & \longrightarrow
\end{array}\right)(\boldsymbol{Y}-\boldsymbol{X} \hat{\boldsymbol{\beta}})=\left(\begin{array}{c}
0 \\
0 \\
\vdots \\
0
\end{array}\right)
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\end{array}\right)(\boldsymbol{Y}-\boldsymbol{X} \hat{\boldsymbol{\beta}})=\left(\begin{array}{c}
0 \\
0 \\
\vdots \\
0
\end{array}\right) \\
\\
\boldsymbol{X}^{T}(\boldsymbol{Y}-\boldsymbol{X} \hat{\boldsymbol{\beta}})=\mathbf{0} .
\end{gathered}
$$

Now we can solve for $\hat{\boldsymbol{\beta}}$ !

Solving for $\hat{\boldsymbol{\beta}}$

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

Inference for $\boldsymbol{\beta}$ (not $\hat{\boldsymbol{\beta}}$ )

## Covariance matrix of the estimators

$$
\operatorname{Cov}(\hat{\boldsymbol{\beta}})=\left(\begin{array}{cccc}
\operatorname{Var}\left(\hat{\boldsymbol{\beta}}_{0}\right) & \operatorname{Cov}\left(\hat{\boldsymbol{\beta}}_{0}, \hat{\boldsymbol{\beta}}_{1}\right) & \ldots & \ldots \\
\operatorname{Cov}\left(\hat{\boldsymbol{\beta}}_{0}, \hat{\boldsymbol{\beta}}_{1}\right) & \operatorname{Var}\left(\hat{\boldsymbol{\beta}}_{1}\right) & \ldots & \ldots \\
\vdots & \vdots & \ddots & \vdots
\end{array}\right)
$$

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\end{array}\right) \\
& =\sigma^{2}\left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-1}
\end{aligned}
$$

Since $\sigma$ is unknown, we use $R S E$ to estimate $\sigma$ :

$$
\mathrm{RSE}=\sqrt{\frac{R S S}{n-p-1}} .
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What we will use instead of $\operatorname{Cov} \hat{\boldsymbol{\beta}}$ is

$$
\widehat{\operatorname{Cov}}(\hat{\boldsymbol{\beta}})=\operatorname{RSE}^{2}\left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-1}
$$

## Example

In the following regression:

$$
\widehat{\text { sales }}=\hat{\beta}_{0}+\hat{\beta}_{1} \times T V+\hat{\beta}_{2} \times \text { radio }+\hat{\beta}_{3} \times \text { newspaper }
$$

We have $\left(\hat{\beta}_{0}, \hat{\beta}_{1}, \hat{\beta}_{2}, \hat{\beta}_{3}\right)=(2.939,0.046,0.189,-0.001)$

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$$

We have $\left(\hat{\beta}_{0}, \hat{\beta}_{1}, \hat{\beta}_{2}, \hat{\beta}_{3}\right)=(2.939,0.046,0.189,-0.001)$
RSE $=\sqrt{\text { RSS } /(n-3-1)}=1.69$ and
$C=\left(\begin{array}{cccc}9.7 \times 10^{-2} & -2.7 \times 10^{-4} & -1.1 \times 10^{-3} & -6.0 \times 10^{-4} \\ -2.7 \times 10^{-4} & 1.9 \times 10^{-6} & -4.5 \times 10^{-7} & -3.3 \times 10^{-7} \\ -1.1 \times 10^{-3} & -4.5 \times 10^{-7} & 7.4 \times 10^{-5} & -1.8 \times 10^{-5} \\ -5.9 \times 10^{-4} & -3.3 \times 10^{-7} & -1.8 \times 10^{-5} & 3.4 \times 10^{-5}\end{array}\right)$
$\operatorname{SE}\left(\hat{\beta}_{3}\right)=$.

## 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

Suppose we want to test between two hypotheses:
$H_{0}:$ None of $\boldsymbol{X}_{1}, \ldots, \boldsymbol{X}_{p}$ is related to $\boldsymbol{Y}$
$H_{a}$ : at least one of $\boldsymbol{X}_{1}, \ldots, \boldsymbol{X}_{p}$ is related to $\boldsymbol{Y}$

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\end{aligned}
$$

This is the same as

$$
\begin{aligned}
& H_{0}: \beta_{1}=\beta_{2}=\ldots=\beta_{p}=0 \\
& H_{a}: \text { at least one of } \beta_{1}, \ldots, \beta_{p} \text { is non-zero. }
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## Relationship between the response and the predictors

Hypothesis test:

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\end{aligned}
$$

The decision will based on the following $F$-statistic:

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

Recall that TSS $=\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}$ and RSS $=\sum_{i=1}^{n}\left(y_{i}-\hat{y}_{i}\right)^{2}$.

## How should we look at $F$ - statistic?

$$
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Provided that $H_{0}$ is true,

$$
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- 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.


## Sales data

$$
\widehat{\text { sales }}=\hat{\beta}_{0}+\hat{\beta}_{1} \times T V+\hat{\beta}_{2} \times \text { radio }+\hat{\beta}_{3} \times \text { newspaper }
$$

- 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 single predictor

The hypothesis test is

$$
\begin{aligned}
& H_{0}: \beta_{j}=0 \\
& H_{a}: \beta_{j} \neq 0
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$$

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$$

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

$$
t=\frac{\hat{\beta}_{j}-0}{\operatorname{SE}\left(\hat{\beta}_{j}\right)}
$$

Here, $\operatorname{SE}\left(\hat{\beta}_{j}\right)$ is the square root of entry $(j, j)$ of $\widehat{\operatorname{Cov}}(\hat{\boldsymbol{\beta}})$, which is an estimate of the covariance matrix of the coefficients.

## 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 | $<0.0001$ |

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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.

## $F$-statistic vs $t$-statistic

Why do we prefer $F$-statistic over $t$-statistic when testing $\beta_{0}=\beta_{1}=\ldots, \beta_{p}=0$ ?

- Calculating $F$ one time is easier than calculating $t$ for $\beta_{0}, \beta_{1}, \ldots, \beta_{p}$.


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Why do we prefer $F$-statistic over $t$-statistic when testing $\beta_{0}=\beta_{1}=\ldots, \beta_{p}=0$ ?

- Calculating $F$ one time is easier than calculating $t$ for $\beta_{0}, \beta_{1}, \ldots, \beta_{p}$.
- If we perform the $t$-test at significance level $\alpha=0.05$ for $\beta_{0}=\beta_{1}=\ldots, \beta_{p}=0$ the probability of us being wrong is:


## Variable selection

## Forward selection:

1. Start with 0 variable. In each step: add a variable that results in the lowest RSS.

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## Backward selection:

1. Start with all variables. In each step: remove a variable with the largest $p$-value.
2. Stop when all $p$-values are below some threshold e.g. 0.001 .

## Model evaluation

- Residual standard error (RSE):

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

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

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

## Example

| Predictos | RSE | $R^{2}$ |
| :--- | :---: | :---: |
| 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.

