# Simple Linear Regression (single variable)

## Introduction to Machine Learning

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January 31, 2017

Some of the figures in this presentation are taken from ”An Introduction to Statistical Learning, with applications in R” (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

# Last Class

1. Basic machine learning framework

$$Y = f(X)$$

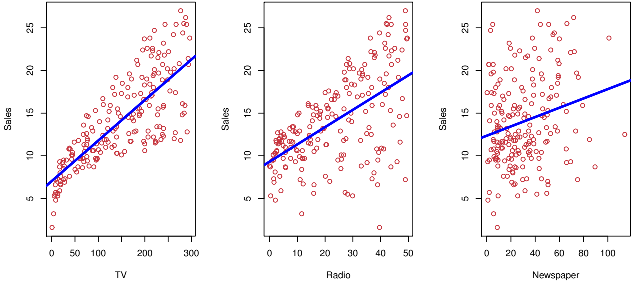
2. Prediction vs inference: predict $Y$ vs understand $f$
3. Parametric vs non-parametric: linear regression vs k-NN
4. Classification vs regressions: k-NN vs linear regression
5. Why we need to have a test set: overfitting

# What is Machine Learning

- Discover unknown function $f$:

$$Y = f(X)$$

- $X$ = set of features, or inputs
- $Y$ = target, or response




$$\text{Sales} = f(\text{TV}, \text{Radio}, \text{Newspaper})$$

# Errors in Machine Learning: World is Noisy

- World is too complex to model precisely
- Many features are not captured in data sets
- Need to allow for errors $\epsilon$ in $f$:

$$Y = f(X) + \epsilon$$

# How Good are Predictions?

- Learned function $\hat{f}$
- Test data: $(x_1, y_1), (x_2, y_2), \ldots$
- **Mean Squared Error (MSE)**:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

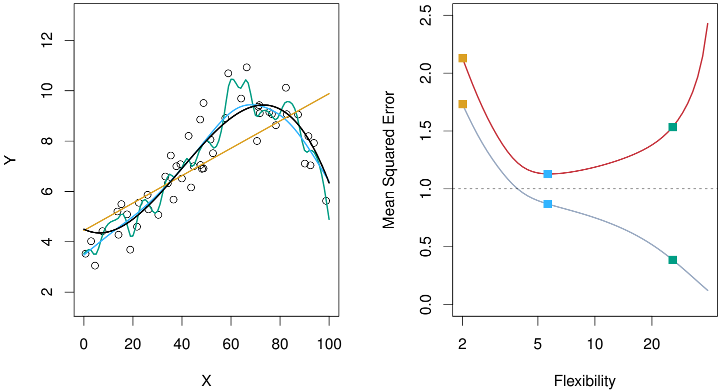
- This is the estimate of:

$$\text{MSE} = \mathbb{E}[(Y - \hat{f}(X))^2] = \frac{1}{|\Omega|}\sum_{\omega\in\Omega}(Y(\omega) - \hat{f}(X(\omega)))^2$$

- Important: Samples $x_i$ are i.i.d.

# Do We Need Test Data?

- Why not just test on the training data?

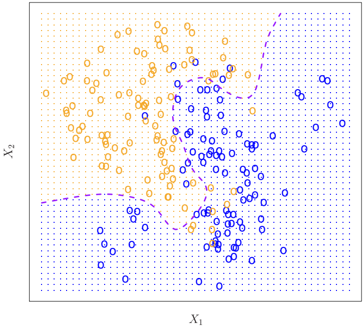



- Flexibility is the degree of polynomial being fit
- Gray line: training error, red line: testing error

# Types of Function $f$

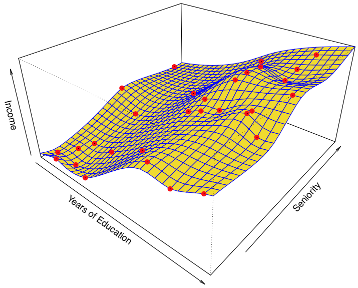
**Classification**: discrete target

$$f : \mathcal{X} \to \{1, 2, 3, \ldots, k\}$$




**Regression**: continuous target

$$f : \mathcal{X} \to \mathbb{R}$$



# Today

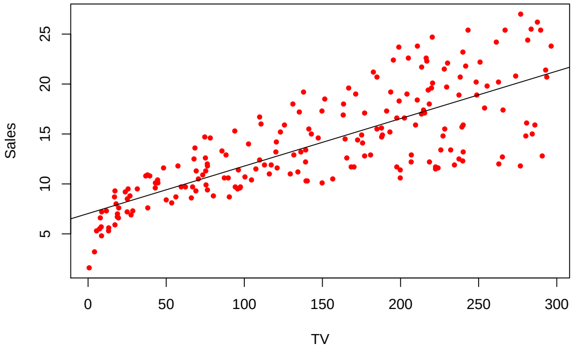
- Basics of linear regression
- Why linear regression
- How to compute it
- Why compute it

# Simple Linear Regression

- We have only one feature

$$Y \approx \beta_0 + \beta_1 X \qquad Y = \beta_0 + \beta_1 X + \epsilon$$

- Example:




$$\text{Sales} \approx \beta_0 + \beta_1 \times \text{TV}$$

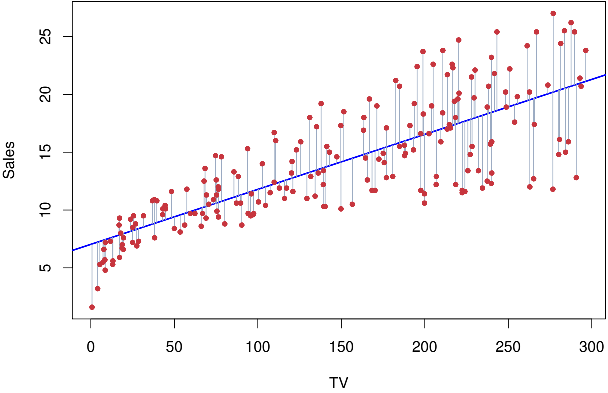
# How To Estimate Coefficients

- No line that will have no errors on data $x_i$
- Prediction:

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- Errors ($y_i$ are true values):

$$e_i = y_i - \hat{y}_i$$



# Residual Sum of Squares

- Residual Sum of Squares

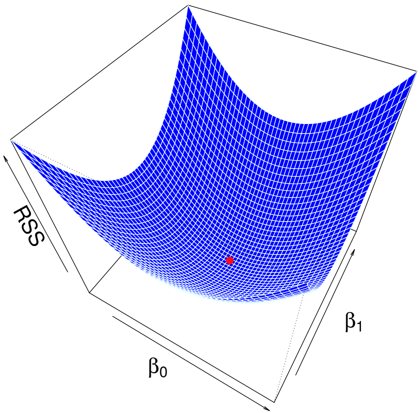
$$\mathrm{RSS} = e_1^2 + e_2^2 + e_3^2 + \cdots + e_n^2 = \sum_{i=1}^{n} e_i^2$$

- Equivalently:

$$\mathrm{RSS} = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

# Minimizing Residual Sum of Squares

$$\min_{\beta_0,\beta_1} \text{RSS} = \min_{\beta_0,\beta_1} \sum_{i=1}^{n} e_i^2 = \min_{\beta_0,\beta_1} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$



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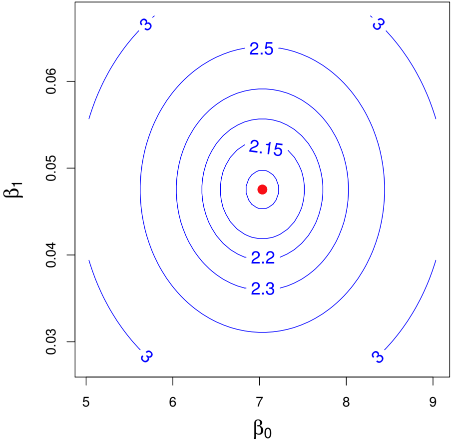

# Solving for Minimal RSS

$$\min_{\beta_0,\beta_1} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

- $\mathrm{RSS}$ is a **convex** function of $\beta_0, \beta_1$
- Minimum achieved when (recall the chain rule):

$$\frac{\partial\,\mathrm{RSS}}{\partial \beta_0} = -2 \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) = 0$$

$$\frac{\partial\,\mathrm{RSS}}{\partial \beta_1} = -2 \sum_{i=1}^{n} x_i (y_i - \beta_0 - \beta_1 x_i) = 0$$

# Linear Regression Coefficients

$$\min_{\beta_0,\beta_1} \sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2$$

Solution:

$$\begin{aligned}
\beta_0 &= \bar{y} - \beta_1 \bar{x} \\
\beta_1 &= \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \frac{\sum_{i=1}^{n} x_i(y_i - \bar{y})}{\sum_{i=1}^{n} x_i(x_i - \bar{x})}
\end{aligned}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

# Why Minimize RSS

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# Why Minimize RSS

1. Maximize likelihood when $Y = \beta_0 + \beta_1 X + \epsilon$ when $\epsilon \sim \mathcal{N}(0, \sigma^2)$
2. Best Linear Unbiased Estimator (BLUE): Gauss-Markov Theorem (ESL 3.2.2)
3. It is convenient: can be solved in closed form

# Bias in Estimation

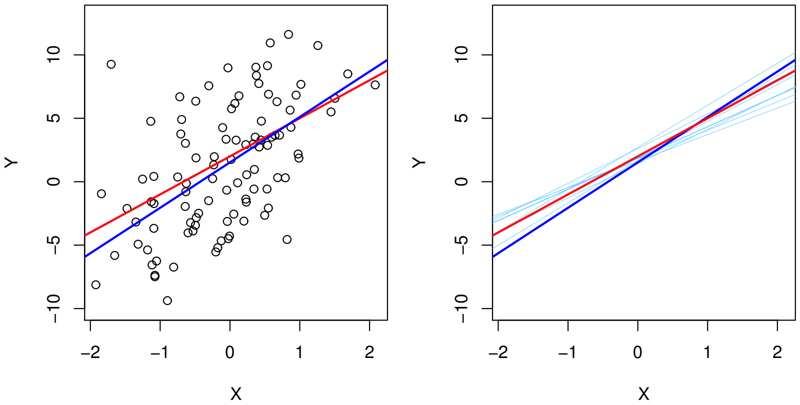
- Assume a true value $\mu^\star$
- Estimate $\mu$ is **unbiased** when $\mathbb{E}[\mu] = \mu^\star$
- Standard mean estimate is unbiased (e.g. $X \sim \mathcal{N}(0,1)$):

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] = 0$$

- Standard variance estimate is biased (e.g. $X \sim \mathcal{N}(0,1)$):

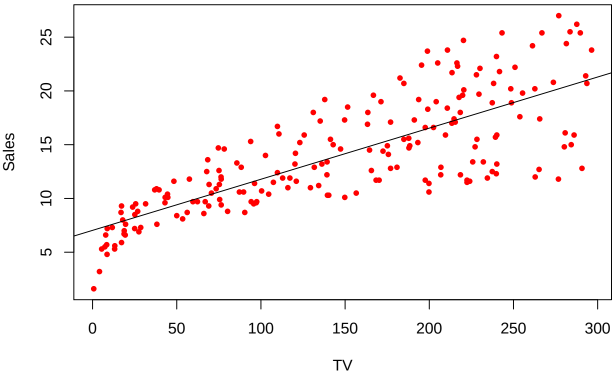
$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2\right] \neq 1$$

# Linear Regression is Unbiased




Gauss-Markov Theorem (ESL 3.2.2)

# Solution of Linear Regression



# How Good is the Fit

- How well is linear regression predicting the training data?
- Can we be sure that TV advertising really influences the sales?
- What is the probability that we just got lucky?

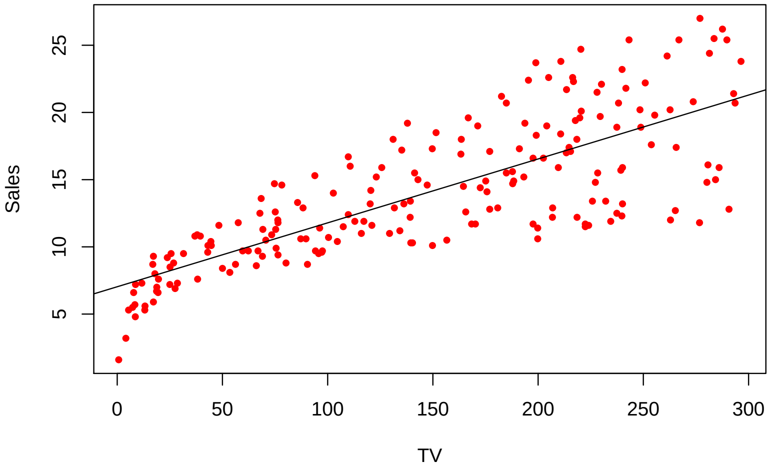
# $R^2$ Statistic

$$R^2 = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

- RSS - residual sum of squares, TSS - total sum of squares
- $R^2$ measures the goodness of the fit as a proportion
- Proportion of data variance explained by the model
- Extreme values:

  0: Model does not explain data
  1: Model explains data perfectly

# Example: TV Impact on Sales



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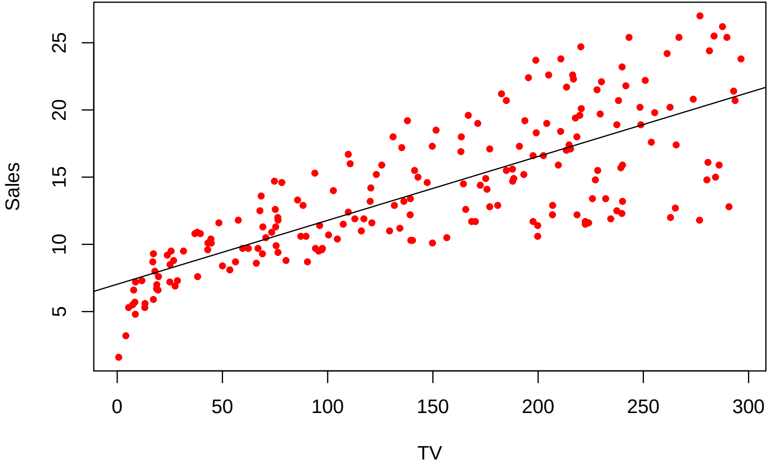
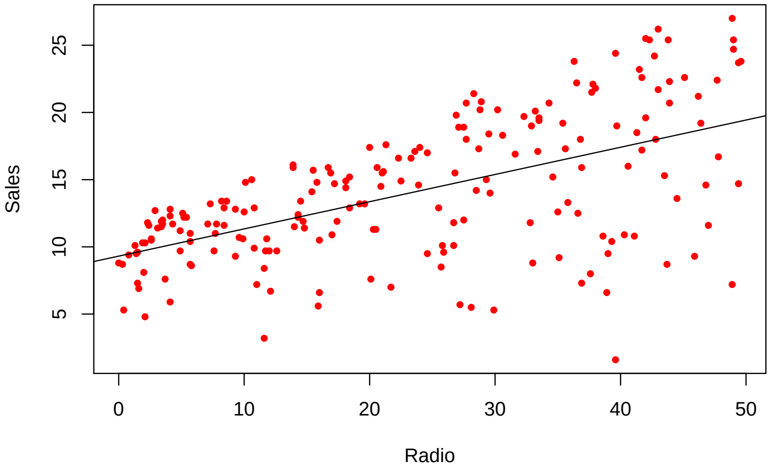



$$R^2 = 0.61$$

# Example: Radio Impact on Sales



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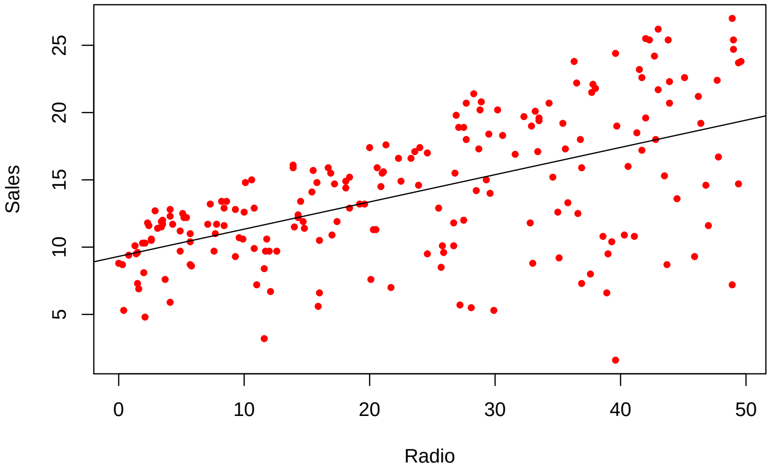
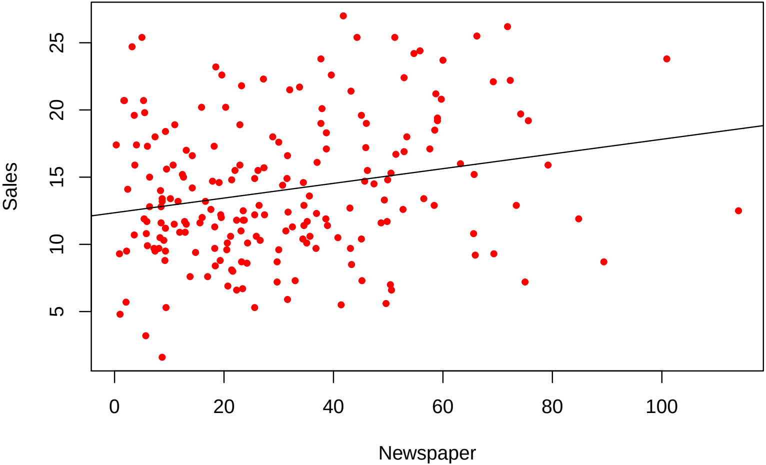
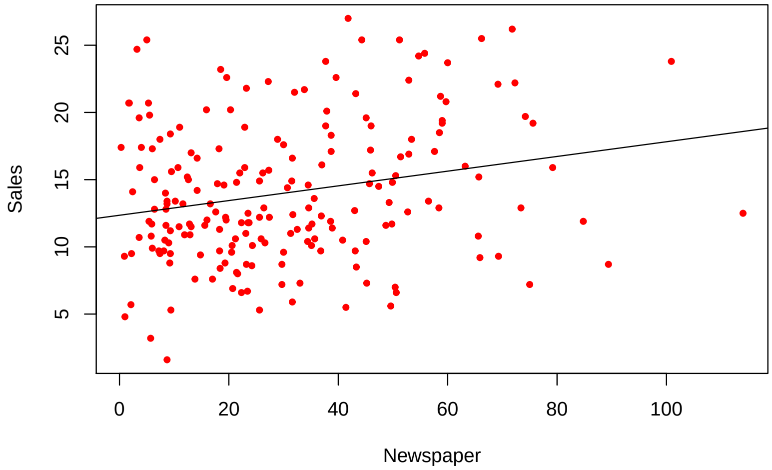



$$R^2 = 0.33$$

# Example: Newspaper Impact on Sales



# Example: Newspaper Impact on Sales




$$R^2 = 0.05$$

# Correlation Coefficient

- Measures dependence between two random variables $X$ and $Y$

$$r = \frac{\mathrm{Cov}(X, Y)}{\sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}}$$

- Like $R^2$ it is between 0,1

  0: Variables are not related
  1: Variables are perfectly related (same)

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- $R^2 = r^2$

# Hypothesis Testing

- Null hypothesis $H_0$:

$$\text{There is no relationship between } X \text{ and } Y$$
$$\beta_1 = 0$$

- Alternative hypothesis $H_1$:

$$\text{There is some relationship between } X \text{ and } Y$$
$$\beta_1 \neq 0$$

- Seek to reject hypothesis $H_0$ with small “probability” ($p$-value) of making a mistake
- Important topic, but beyond the scope of the course

# Multiple Linear Regression

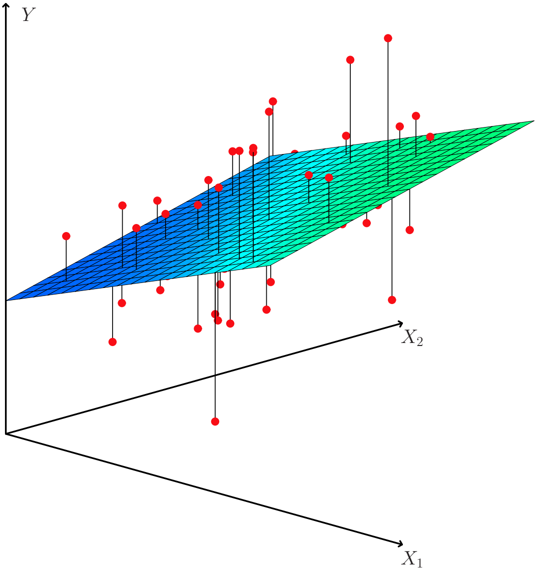
- Usually more than one feature is available

$$\text{sales} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_3 \times \text{newspaper} + \epsilon$$

- In general:

$$Y = \beta_0 + \sum_{j=1}^{p} \beta_j X_j$$

# Multiple Linear Regression



# Estimating Coefficients

- Prediction:

$$\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_{ij}$$

- Errors ($y_i$ are true values):

$$e_i = y_i - \hat{y}_i$$

- Residual Sum of Squares

$$\mathrm{RSS} = e_1^2 + e_2^2 + e_3^2 + \cdots + e_n^2 = \sum_{i=1}^{n} e_i^2$$

- How to minimize RSS? Linear algebra!

# Linear Regression Answers

1. Are predictors $X_1, X_2, \ldots, X_p$ really predicting $Y$?
2. Is only a subset of predictors useful?
3. How well does linear model fit data?
4. What $Y$ should be predict and how accurate is it?

# Answer 1

"Are predictors $X_1, X_2, \ldots, X_p$ really predicting $Y$?"

- Null hypothesis $H_0$:

  There is no relationship between $X$ and $Y$

  $$\beta_1 = 0$$

- Alternative hypothesis $H_1$:

  There is some relationship between $X$ and $Y$

  $$\beta_1 \neq 0$$

- Seek to reject hypothesis $H_0$ with small "probability" ($p$-value) of making a mistake
- See ISL 3.2.2 on how to compute F-statistic and reject $H_0$

# Answer 2

"Is only a subset of predictors useful?"

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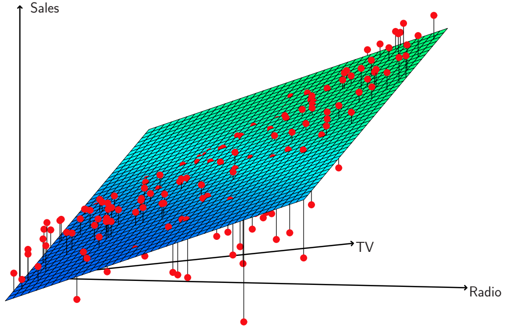
- Testing all subsets of features is impractical: $2^p$ options!
- More on how to do this later

# Answer 3

"How well does linear model fit data?"

- $R^2$ also always increases with more features (like RSS)
- Is the model linear? Plot it:




- More on this later

# Answer 4

"What $Y$ should be predict and how accurate is it?"

- The linear model is used to make predictions:

$$y_{\text{predicted}} = \hat{\beta}_0 + \hat{\beta}_1\, x_{\text{new}}$$

- Can also predict a confidence interval (based on estimate on $\epsilon$):
- Example:
  - Spent $\$100\,000$ on TV advertising
  - Spent $\$20\,000$ on Radio advertising
  - Confidence interval $[10.985, 11, 528]$ - predict $f(X)$ (the average response)
  - Prediction interval $[7.930, 14.580]$ - predict $f(X) + \epsilon$ (response + possible noise)

R notebook