Introduction to Machine Learning

Lecture 4
Linear Models I

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26 – 30 November 2018
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Types of learning problems

Supervised learning	Unsupervised learning	Reinforcement learning
Learning from supervision (i.e., teacher) Given inputs and **outputs**, learn a function that maps input → output	Learning with no supervision Given only inputs, extract some pattern from the data.	Learning from rewards and punishments. Inspired by (operant) conditioning in psychology. The agent acts in an environment over some **time**. It gets reward/punishment from time to time. Needs to learn a *policy* to maximize reward.
Examples: - Recognizing faces - Predicting the sales for a product - Learning to rank search results	Examples: - Clustering (market segmentation) - Dimensionality reduction (visualization) - Generating celebrity faces	Examples: - Most robotics applications (e.g. learning to move around) - Playing games (e.g., AlphaGo)

Supervised learning

- Two main types of problems
  - Regression
    - Outputs are real-valued (quantitative)
    - Examples:
      - Predicting the sales of a product
      - Predicting the value of a home
  - Classification
    - Outputs are discrete (qualitative)
    - Examples:
      - Face/speech/object recognition
      - Predicting if a person will default on their loan
      - Predicting whether a stock will go up or down

- *Note inputs can be of any type (real-valued or discrete).*

Linear regression

- Assume the relation between input and output is linear

$$y = \beta_0 + \sum_{d=1}^{D} x_d \beta_d$$

- β are known as parameters or coefficients
- β_0 is known as bias or intercept

- Matrix notation
  - $X_{N \times (D+1)}$: Data matrix. N samples. D features (measurements)
    - Add a new feature (column) that is all 1s.
  - Y_N: Output (target) vector. N samples.
  - β_D: Parameter vector. D coefficients.
  - Then, the above can be written as

$$Y = X\beta$$

Linear regression

- Note that we can apply any (possibly nonlinear) preprocessing on x

$$y = \beta_0 + \sum_{d=1}^{D} \phi(x_d)\beta_d$$

- This is still a linear model. Because it is **linear in the parameters**.
- Linearity

$$y(c_1\beta + c_2\gamma) = c_1 y(\beta) + c_2 y(\gamma)$$

- Why do we care about linear regression?
  - Easy to interpret
  - May outperform complex models if
    - Little data
    - High noise in data
  - Foundation for many techniques

Solving linear regression

- Find the parameters that fit the training data $\{x, y\}_{n=1,2,\ldots,N}$
  - Pick the *line* that passes as close as possible to the training points
- How do we measure closeness?

$$E(\beta) = \frac{1}{2}\sum_{n=1}^{N}(y - (\beta_0 + \sum_{d=1}^{D} X_{nd}\beta_d))^2$$

- Find parameters that minimize the sum-of-squares error (method of least squares)
  - Set derivative to 0 and solve for β

- For 1D case

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2},$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1\bar{x},$$

$\bar{x}$: Mean of x
$\bar{y}$: Mean of y

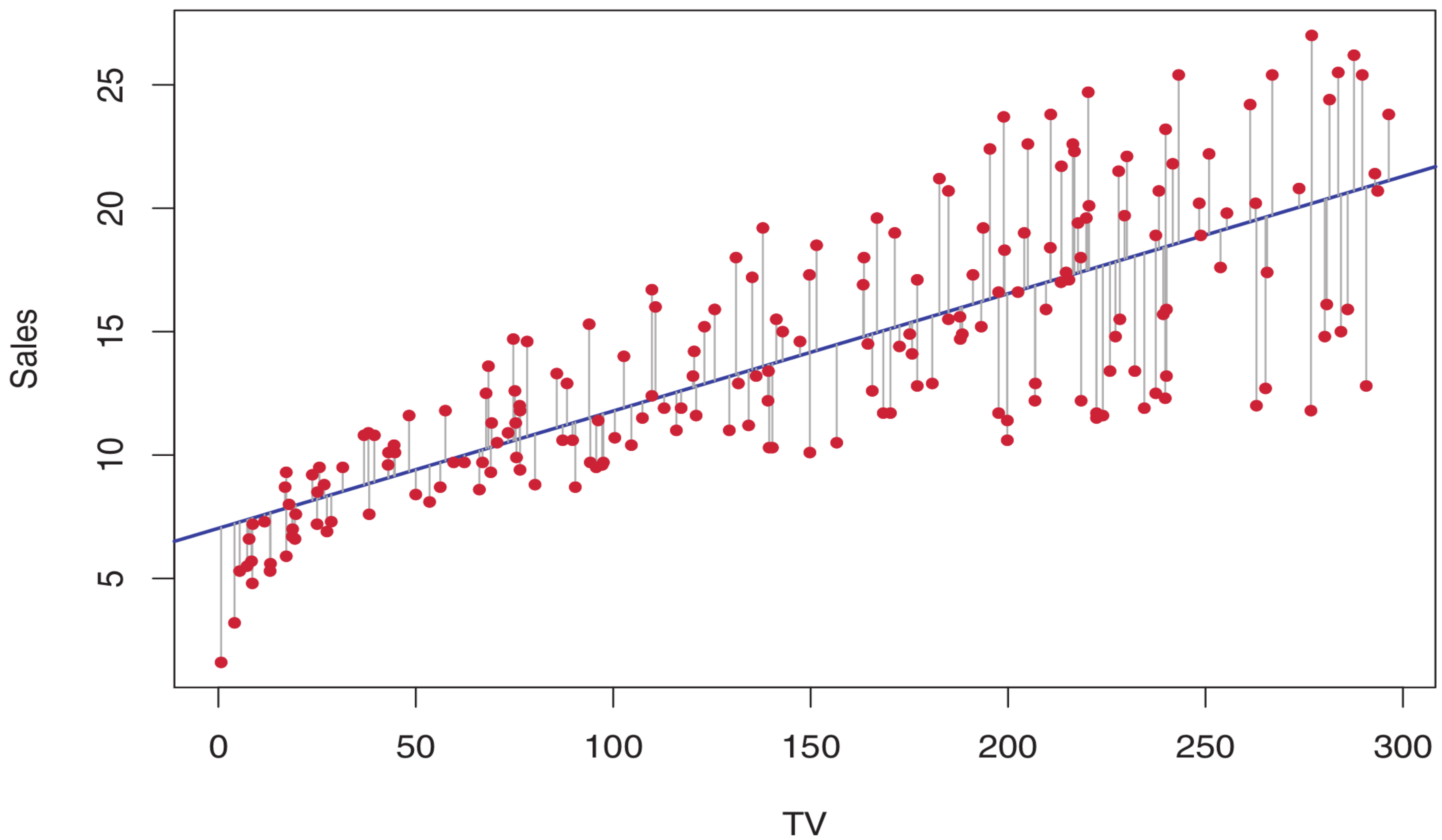


FIGURE 3.1. *For the* `Advertising` *data, the least squares fit for the regression of* `sales` *onto* `TV` *is shown. The fit is found by minimizing the sum of squared errors. Each grey line segment represents an error, and the fit makes a compro-*

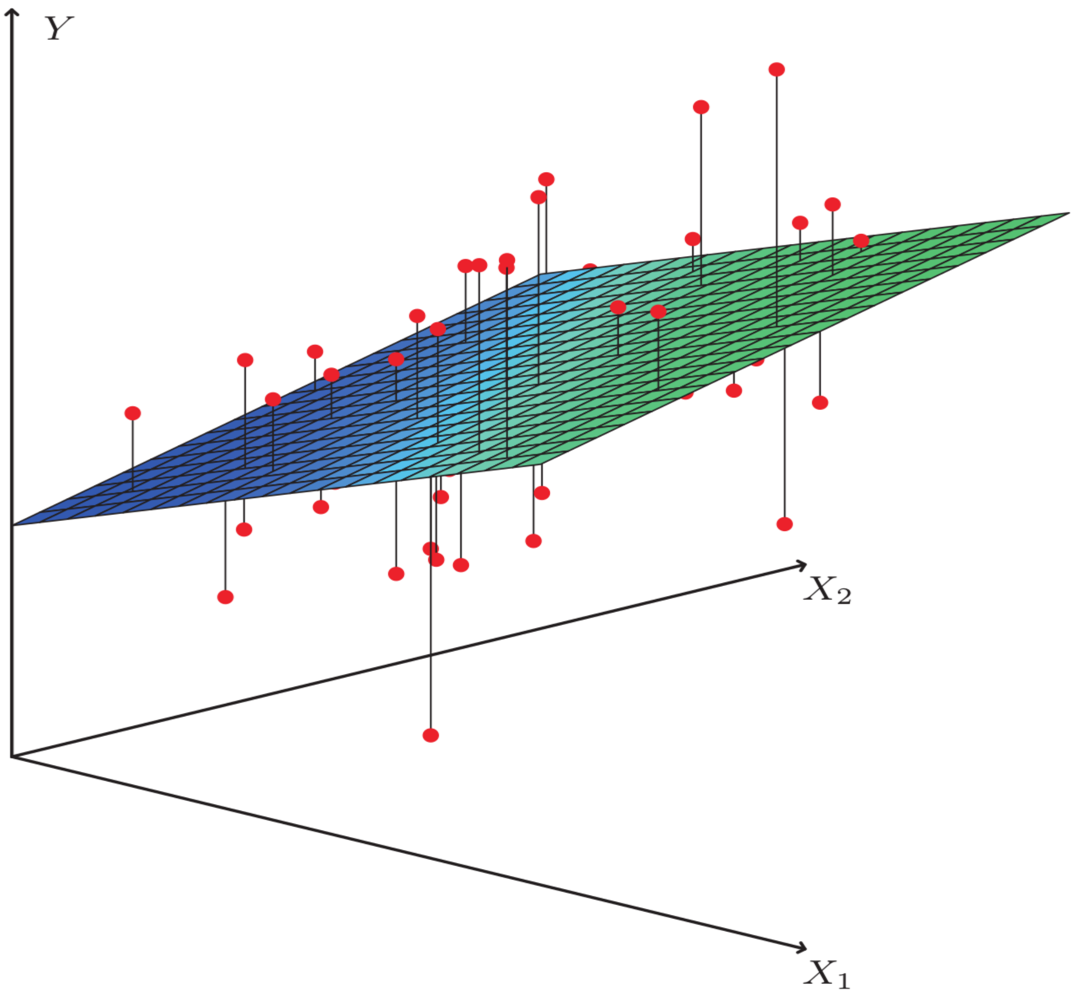


FIGURE 3.4. *In a three-dimensional setting, with two predictors and one response, the least squares regression line becomes a plane. The plane is chosen*

Solving linear regression

- Linear regression is an *easy* problem
  - Convex (i.e., single global minimum)
  - Fast algorithms available

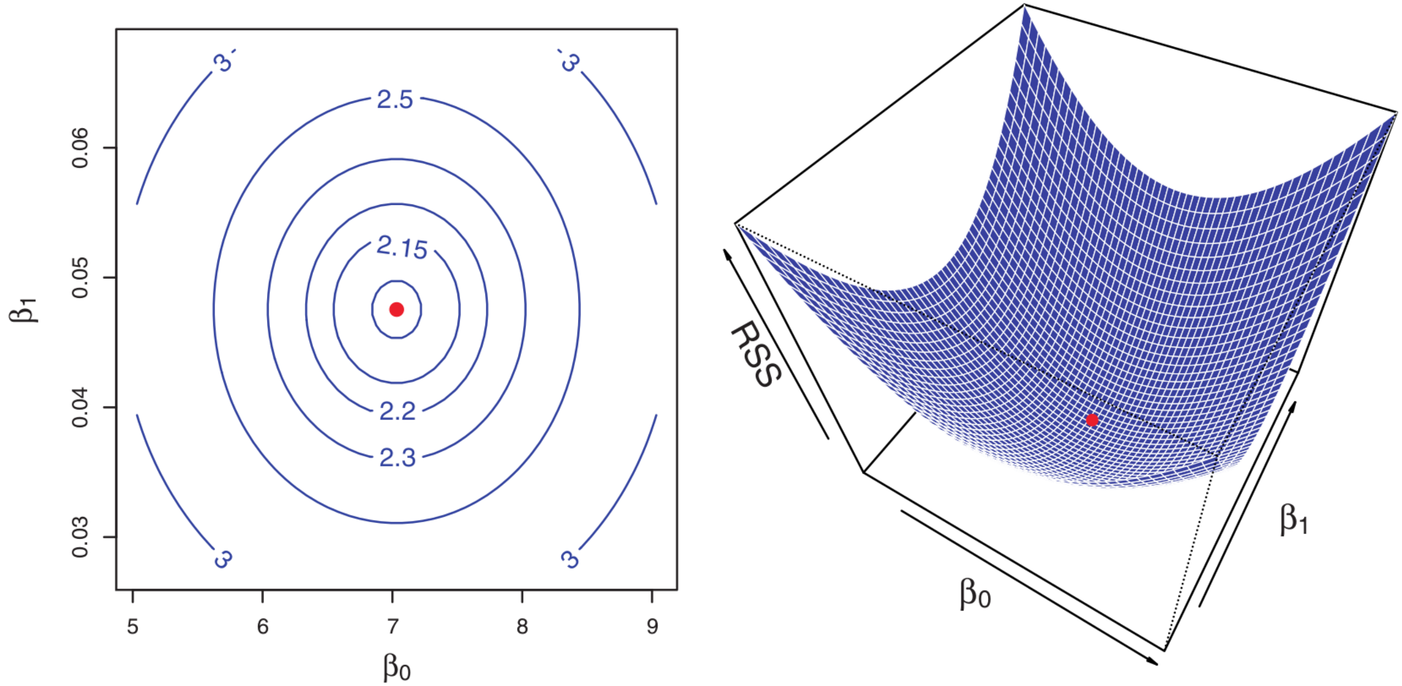


FIGURE 3.2. *Contour and three-dimensional plots of the RSS on the* `Advertising` *data, using* `sales` *as the response and* `TV` *as the predictor. The red dots correspond to the least squares estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, given by (3.4).*

Solving the general case

- Minimize the following wrt to β

$$\mathrm{RSS}(\beta) = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta). \quad (3$$

This is a quadratic function in the $p + 1$ parameters. Differentiating wi respect to β we obtain

$$\frac{\partial \mathrm{RSS}}{\partial \beta} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta)$$

$$\frac{\partial^2 \mathrm{RSS}}{\partial \beta \partial \beta^T} = 2\mathbf{X}^T\mathbf{X}. \quad (3$$

Assuming (for the moment) that $\mathbf{X}$ has full column rank, and hence $\mathbf{X}^T$

- Need to assume that X is full rank (no linearly dependent columns)
- The solution is

$$\frac{\partial^2 \mathrm{RSS}}{\partial \beta \partial \beta^T} = 2\mathbf{X}^T\mathbf{X}.$$

or the moment) that $\mathbf{X}$ has full column rank, and

efinite, we set the first derivative to zero

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

e unique solution

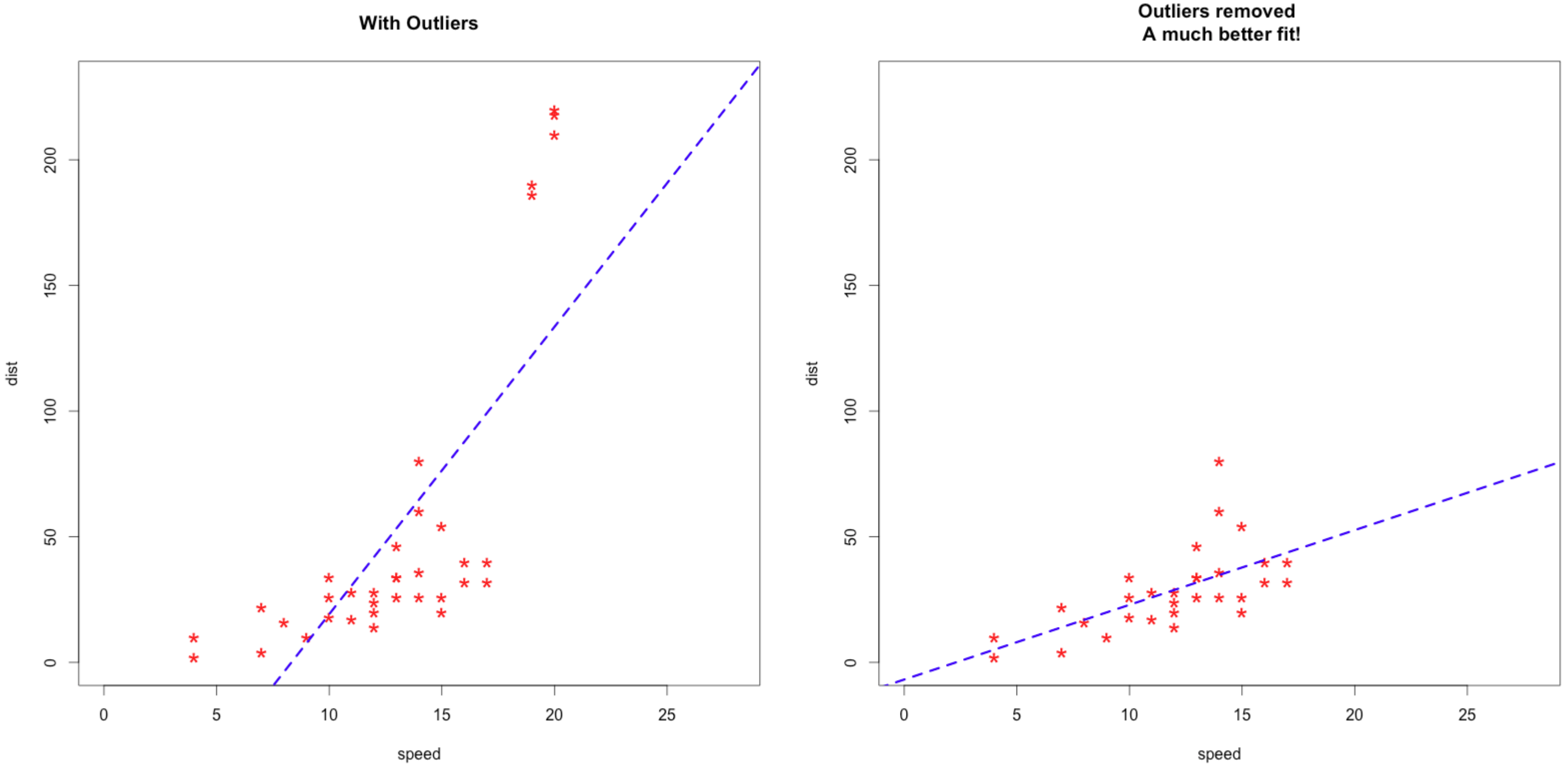
$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}.$$

- In python, `numpy.linalg.lstsq`
- In R, `fit ← lm(y ~ x1 + x2 + x3 ...)`

- Good resources for matrix calculus
  - http://www.matrixcalculus.org/
  - https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

What can go wrong?

- Outliers



[3]

- Robust alternatives
  - Use absolute value instead of squared error
  - Harder to solve

What can go wrong?

- Correlated inputs (colinearity)

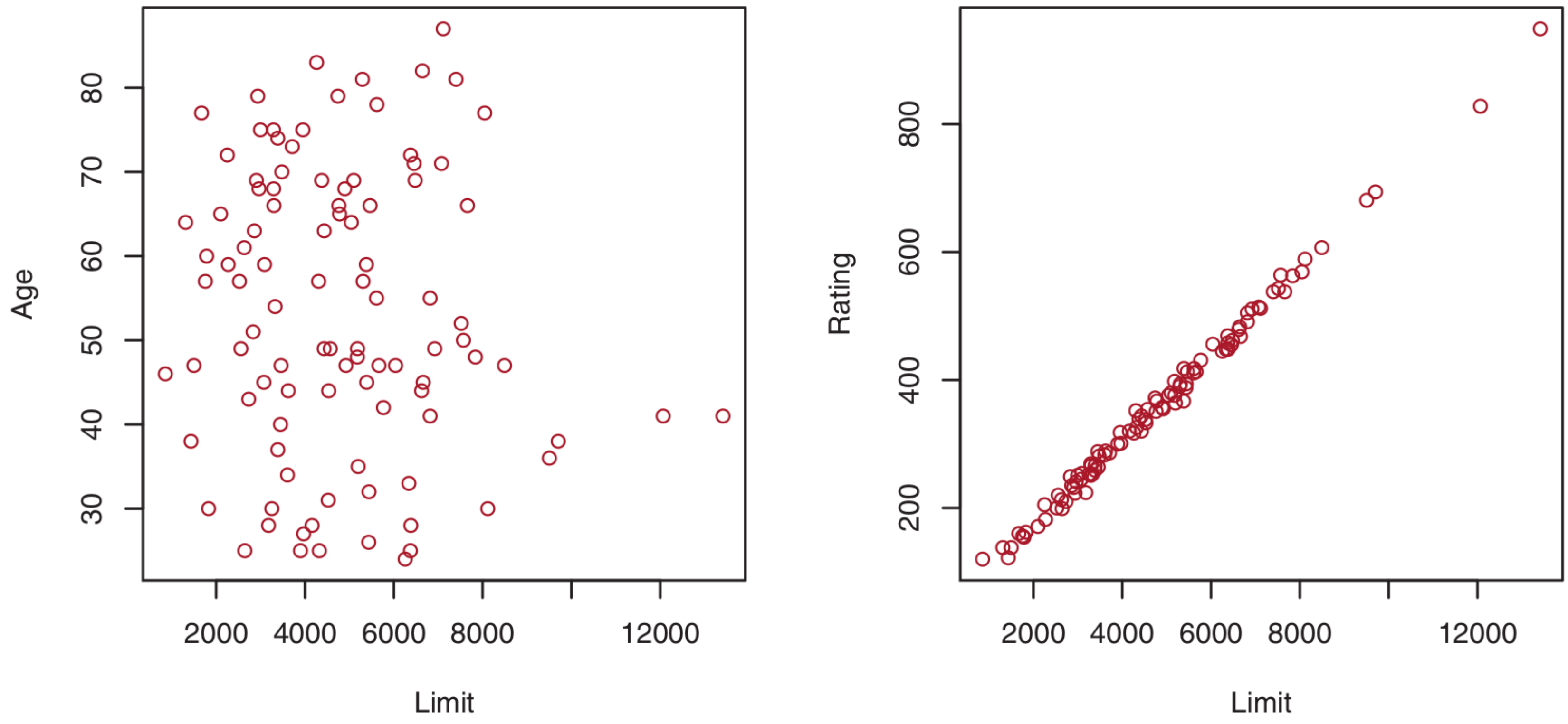


FIGURE 3.14. *Scatterplots of the observations from the* `Credit` *data set.* Left: *A plot of* `age` *versus* `limit`*. These two variables are not collinear.* Right: *A plot of* `rating` *versus* `limit`*. There is high collinearity.*

What can go wrong?

- Correlated inputs (colinearity)
  - Solution unstable
  - Hard to interpret
  - What can we do?
    - Look at the correlation matrix
    - Whiten input data (PCA)

- Correlation of error-terms
  - Violates the independence assumption
  - e.g., Time-series data

What can go wrong?

- Nonlinear input – output relation
  - Interaction terms
  - Residual (error) plot

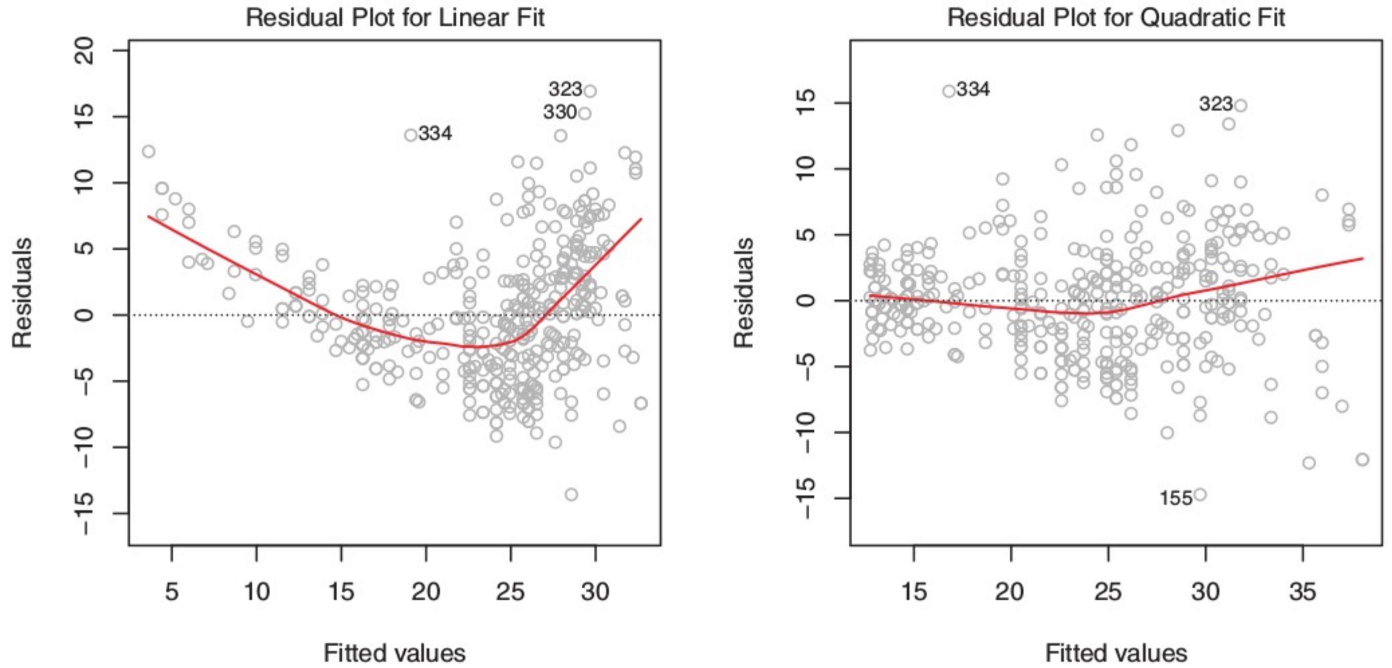


FIGURE 3.9. *Plots of residuals versus predicted (or fitted) values for the* `Auto` *data set. In each plot, the red line is a smooth fit to the residuals, intended to make it easier to identify a trend.* Left: *A linear regression of* `mpg` *on* `horsepower`*. A strong pattern in the residuals indicates non-linearity in the data.* Right: *A linear regression of* `mpg` *on* `horsepower` *and* `horsepower`^{2}*. There is little pattern in the residuals.*

Summary

- Linear regression
  - Formulation
  - How to solve it
  - What can go wrong

- Exercises
  - Solve 1D case
  - Do the lab in Section 3.6 of ISLR

References

[1] James, Witten, Hastie, and Tibshirani. An Introduction to Statistical Learning with Applications in R. Chapter 3.

[2] Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning. Chapter 3.

[3] http://r-statistics.co/Outlier-Treatment-With-R.html