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5. Linear Regression

Data Analysis for Networks - DataNets'19
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Bibliography

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☞ Chapter 3
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B.2 H. Pishro-Nik, ”Introduction to probability, statistics, and random processes”, available at https://www.probabilitycourse.com, Kappa Research LLC, 2014.

Intro

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Linear Regression: A very simple approach for Supervised Learning:
- been around for a very long time...
- predicts a quantitative response.
- explains the relationship between two or more variables.

Many fancy statistical learning approaches can be seen as generalisation or extensions of linear regression.

This lecture: Linear Regression, Least-Squares

Some history

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- (**1875**) Sir Francis Galton originally conceived modern notions of correlation and regression, by studying eugenics of sweet pea seeds.
- (**1896**) Karl Pearson publishes the first rigorous treatment of correlation and regression in the *Philosophical Transactions of the Royal Society of London*.
- (**1981**) E.E. Ghiselli presents a simple proof of optimality of regression related to the sum of squared errors.

Source
Galton, Pearson, and the Peas: A Brief History of Linear Regression for Statistics Instructors, by Jeffrey M. Stanton (2017)

It all started like this...

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Training data available:

$$D_n \quad = \quad \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$$

Data come in pairs $(\mathbf{x}_i, y_i)$ of

- $\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,K})$ input data, as a vector of size $K \geq 1$.
- y_i output data of size 1.

Goal: Given set of known I/O pairs, "guess" a function $f : \mathbb{R}^K \rightarrow \mathbb{R}$ that for any input $\mathbf{x^{(o)}}$ predicts its output $y^{(o)}$.

☞ We hope to get a "good" prediction. What is "good"?

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We are looking for an expression

$$y = f(x_1, \ldots, x_K) + \epsilon$$

which can express the output y as a deterministic function of the input $\mathbf{x} = (x_1, \ldots, x_K)$ plus an additive random perturbation ϵ from some distribution (usually white noise $\mathcal{N}(0, \sigma^2)$).

☞ In this way we can do predictions of unknown output, given any input.

We will try to **estimate** the function $f(x_1, \ldots, x_K)$ using the existing training data.

Linear Regression

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Linear Regression: **Assumes** that the output is an affine function of the input

$$y = \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_K x_K + \beta_0 + \epsilon. \quad (1)$$

Unknowns:
- $(\beta_1, \ldots, \beta_K) \in \mathbb{R}^K$ is a vector of *parameters/coefficients*.
- β_0 is the *bias parameter or intercept*.
- ϵ is a random error term; independent of $\mathbf{x}$ with mean 0.

☞ Using known pairs, find the Regression line = "line of best fit".

Simple Linear Regression

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Let us simplify for just 1-dimension, $x \in \mathbb{R}$.

$$y = \beta_1 x + \beta_0 + \epsilon \tag{2}$$

- β_1 is the slope (average increase in y for unit increase of x).
- β_0 is the intercept term (expected value of y when $x = 0$),
- ϵ is the error term, which summarises what we miss by using a simple linear model, e.g. non-linearities, other variables, or measurement errors.

Simple Linear Regression, cont'd

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Simple Goal: Use training data to produce estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients. Then we can make the prediction $\hat{y}_o$ for y_o, on the basis of input x_o:

$$\hat{y} = \hat{\beta}_1 x + \hat{\beta}_0, \quad (3)$$

☞ Draw a line in the $x - y$ plane that best "fits" our data points. This is called the regression line (without the error term).

Examples

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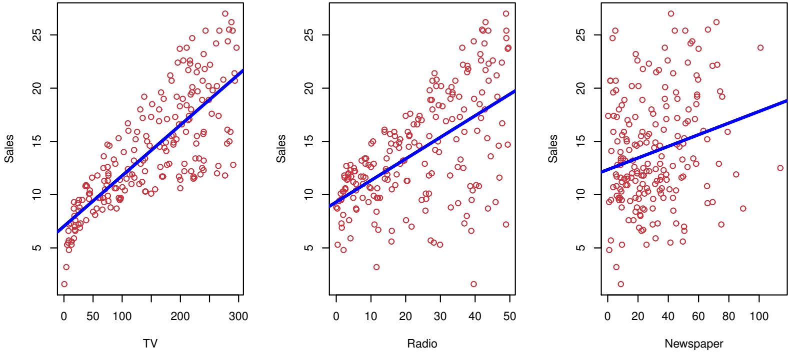

Figure: Advertisement Related Example. [1]

[1] Figure from [B.1] with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

How to draw the line?

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We need to draw a line that "fits well" the known data. How?

- The available known data are the pairs (x_i, y_i), $i = 1, \ldots, n$.
- The regression line gives $\hat{y}_i = \hat{\beta}_1 x_i + \hat{\beta}_0$, for input x_i.

Definition: the following quantities are called residuals

$$\epsilon_i := y_i - \hat{y}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i \quad . \tag{4}$$

Residuals

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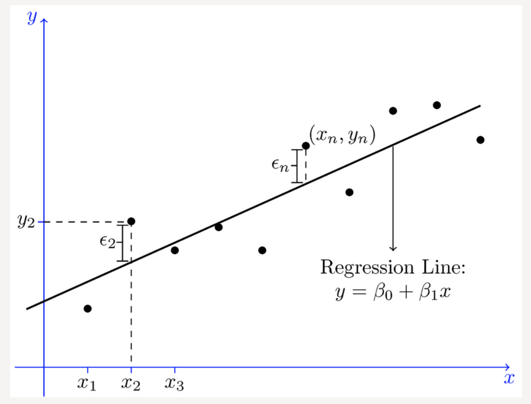

Figure: Regression Line and Residuals.[2]

[2] Source [B.2]

Sum of Squares

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The *Residual Sum of Squares (RSS)* is a function of $\hat{\beta}_0$, $\hat{\beta}_1$,

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

It is always non-negative $RSS \geq 0$.

☞ Find and use the coefficients that minimize the RSS! This should provide a good fit to the data.

Least Squares

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The optimal *least squares coefficient estimates* are found by:

$$\min \quad RSS(\hat{\beta}_0, \hat{\beta}_1).$$

Solution:

$$\begin{aligned} \frac{\partial RSS}{\partial \hat{\beta}_0} &= 2(-1)\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0, \\ \frac{\partial RSS}{\partial \hat{\beta}_1} &= 2(-1)\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)x_i = 0. \end{aligned}$$

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Coefficient Estimates

Given $n \geq 3$ observations $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, we estimate β_0 and β_1 as

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}, \quad (5)$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}, \quad (6)$$

where $\bar{y} := \frac{1}{n} \sum_{i=1}^n y_i$ and $\bar{x} := \frac{1}{n} \sum_{i=1}^n x_i$ are the sample means.

Alternative Method

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Consider again the linear model with random errors.
Error ϵ has zero mean $\mathbb{E}[\epsilon] = 0$ and is independent of x.

$$y = \beta_1 x + \beta_0 + \epsilon$$

☞ Applying expectation on both sides, we get

$$\begin{aligned} \mathbb{E}[y] &= \beta_1 \mathbb{E}[x] + \beta_0 + \mathbb{E}[\epsilon] \\ &= \beta_1 \mathbb{E}[x] + \beta_0. \end{aligned}$$

Alternative Method cont'd

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☞ We take covariance between x and $y = \beta_0 + \beta_1 x + \epsilon$.

$$\begin{aligned} Cov(x,y) &:= \mathbb{E}\left[(x-\mathbb{E}[x])(y-\mathbb{E}[y])\right] \\ &= \mathbb{E}\left[(x-\mathbb{E}[x])(\beta_0+\beta_1 x+\epsilon-\beta_0-\beta_1\mathbb{E}[x]-\mathbb{E}[\epsilon])\right] \\ &= \mathbb{E}\left[(x-\mathbb{E}[x])(\epsilon+\beta_1(x-\mathbb{E}[x])\right] \\ &= \beta_1\mathbb{E}\left[(x-\mathbb{E}[x])^2\right] =: \beta_1 \cdot Var(x) \end{aligned}$$

Alternative Method cont'd II

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$$\beta_1 = \frac{Cov(x,y)}{Var(x)}, \quad (7)$$

$$\beta_0 = \mathbb{E}[y] - \beta_1 \mathbb{E}[x]. \quad (8)$$

☞ With the observed pairs $(x_1, y_1), \ldots, (x_n, y_n)$ we get the estimates $\hat{\beta}_0$, $\hat{\beta}_1$,

$$\mathbb{E}[x] \approx \frac{1}{n}\sum_{i=1}^{n} x_i =: \bar{x}, \quad (9)$$

$$\mathbb{E}[y] \approx \frac{1}{n}\sum_{i=1}^{n} y_i =: \bar{y}, \quad (10)$$

$$Var(x) \approx \frac{1}{n-1}\sum_{i=1}^{n} (x_i - \bar{x})^2 =: s_{xx} \quad (11)$$

$$Cov(x,y) \approx \frac{1}{n-1}\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) := s_{xy} \quad (12)$$

Remark: For s_{xx} and s_{xy}, division by n or $n-1$ does not affect the coefficients. But the same choice should be applied to both estimators.

Numerical Example

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Consider a data set of $n = 4$ known (x, y) samples

$$D_4 = \{(1,3),\ (2,4),\ (3,8),(4,9)\}$$

Find:

- The coefficients $\hat{\beta}_0, \hat{\beta}_1$ for the simple linear regression.
- The residuals ϵ_i from the estimated values.

Solution

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$$\bar{x} = \frac{1+2+3+4}{4} = 2.5 \quad , \quad \bar{y} = \frac{3+4+8+9}{4} = 6.$$

$$s_{xx} = \frac{1}{4-1}\left[(1-2.5)^2 + (2-2.5)^2 + (3-2.5)^2 + (4-2.5)^2\right] = \frac{5}{3}$$

$$s_{xy} = \frac{1}{4-1}\ [(1-2.5)(3-6) + (2-2.5)(4-6) +$$
$$+ (3-2.5)(8-6) + (4-2.5)(9-6)] = \frac{11}{3}$$

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Solution cont'd

$$\hat{\beta}_1 = \frac{s_{xy}}{s_{xx}} = \frac{11}{5} = 2.2$$
$$\hat{\beta}_0 = 6 - (2.2)(2.5) = 0.5$$

Regression-line:

$$\hat{y}_i = 0.5 + 2.2x_i,$$

Residuals:

$$\hat{y}_1 = 2.7,\ \hat{y}_1 = 4.9,\ \hat{y}_1 = 7.1\ \hat{y}_1 = 9.3$$

$$\hat{\epsilon}_1 = 0.3,\ \hat{\epsilon}_2 = -0.9,\ \hat{\epsilon}_3 = 0.9\ \hat{\epsilon}_4 = -0.3$$

☞ Verification: $\hat{\epsilon}_1 + \hat{\epsilon}_2 + \hat{\epsilon}_3 + \hat{\epsilon}_4 = 0$. (Why?)

Accuracy of the model

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- *Mean Squared Error (MSE)*.
- *Residual Standard Error (RSE)*.
- R^2 statistic or *Coefficient of determination*.
- Confidence intervals.
- p-value.

Mean Squared Error

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One can use the Mean Squared Error (MSE), defined as

$$
\begin{aligned}
MSE &:= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 && (13)\\
&= \frac{1}{n}RSS && (14)
\end{aligned}
$$

It is a measure of *lack of fit* for the model.

Residual Standard Error

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The residual standard error provides the average amount that the response y deviates form the true regression line $\beta_0 + \beta_1 x$.

$$RSE = \sqrt{\frac{1}{n-2} RSS} = \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}. \tag{15}$$

It is a measure of *lack of fit* for the model, having also the nice interpretation,

$$Var(\epsilon) \approx RSE^2. \tag{16}$$

R^2 statistic

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✏ An alternative name is Coefficient of determination.

$R^2 \in [0,1]$ is the proportion of variability in y (dependent) that can be explained / predicted by knowing the variability of x (independent).
☞ The closer to 1, the better the fit.

$$\begin{aligned} R^2 &= \frac{Explained \quad Variation}{Total \quad Variation} = 1 - \frac{RSS}{TSS} \\ &= \frac{\beta_1^2 Var(x)}{Var(y)} \overset{(7)}{=} \frac{[Cov(x,y)^2]}{Var(x)Var(y)} \approx \frac{s_{xy}^2}{s_{xx}s_{yy}} =: \rho^2. \end{aligned} \tag{17}$$

☞ In this case equal to ρ^2 the "sample correlation coefficient".

$TSS = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the *Total Sum of Squares*.

R^2 statistic cont'd

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To better understand, let us take a look at the variance of $y = \beta_0 + \beta_1 + \epsilon$,

$$Var(y) \overset{indep. x,\epsilon}{=} \beta_1^2 Var(x) + Var(\epsilon).$$

1. Variance due to variation of x: $\beta_1^2 Var(x)$
2. Variance of error: $Var(\epsilon)$. (Variance left in y after we know x)

☞ If $Var(\epsilon)$ is small, then y will be close to $\beta_0 + \beta_1 x$, so that our linear regression model will successfully estimate y.

R^2 example

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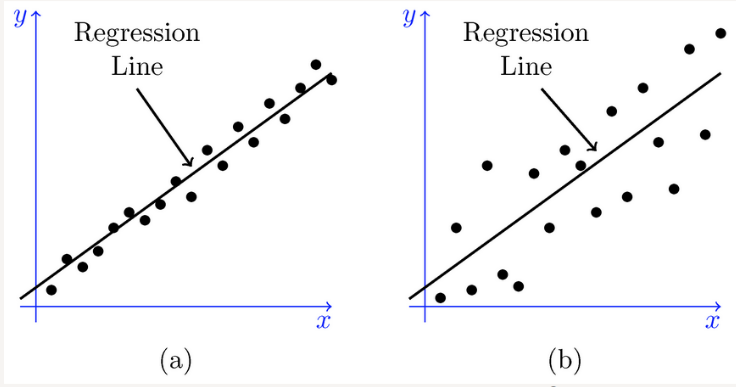

Figure: *left*: high value of R^2, *right*: low value of R^2. [3]

[3] Source [B.2]

Confidence intervals

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The 95% confidence intervals for β_0 and β_1 are

$$\hat{\beta}_0 \pm 2 \cdot SE(\hat{\beta}_0), \quad and \quad \hat{\beta}_1 \pm 2 \cdot SE(\hat{\beta}_1), \tag{18}$$

where SE is the *Standard Error*.

$$SE(\hat{\beta}_0)^2 = Var(\epsilon)\left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right], \tag{19}$$

$$SE(\hat{\beta}_1)^2 = \frac{Var(\epsilon)}{\sum_{i=1}^{n}(x_i - \bar{x})^2}. \tag{20}$$

To estimate $Var(\epsilon)$ we use the *Residual Standard Error (RSE)*

$$Var(\epsilon) \approx RSE^2. \tag{21}$$

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p-value: Are x and y related?

$$H_0 : \beta_1 = 0$$

versus

$$H_1 : \beta_1 \neq 0$$

If $\beta_1 = 0$ then the model reduces to $Y = \beta_0 + \epsilon$, and x is not associated with y.

Q: Given $\hat{\beta}_1 > 0$ what is the probability of this being a false alarm?

☞ To answer, we compute the p-value. This relates to the probability that $\hat{\beta}_1$ is close to 0, related to the standard error.

If the *p-value* is very small ($1\% - 5\%$) we reject the null hypothesis, i.e. a relationship does exist between x and y .

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Numerical Example cont'd

- RSS $= \hat{\epsilon}_1^2 + \hat{\epsilon}_2^2 + \hat{\epsilon}_3^2 + \hat{\epsilon}_4^2 = 0.3^2 + 0.9^2 + 0.9^2 + 0.3^2 = 1.8$
- MSE $= \frac{RSS}{n} = \frac{1.8}{4} = 0.45.$
- RSE $= \sqrt{\frac{RSS}{n-2}} = \sqrt{\frac{1.8}{4-2}} \approx 0.949.$
- $R^2 = \frac{s_{xy}^2}{s_{xx}s_{yy}} = \frac{(11/3)^2}{(5/3)\cdot s_{yy}} = \frac{(11/3)^2}{(5/3)\cdot(26/3)} \approx 0.93.$
- $s_{yy} = \frac{1}{4-1}\left[(3-6)^2 + (4-6)^2 + (8-6)^2 + (9-6)^2\right] = \frac{26}{3}.$

☞ R^2-statistic is 0.93, hence close to 1, and the fit is good!
(Cannot tell just by RSE)

Multiple Linear Regression Model

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Very often, a response depends on several $(K > 1)$ features.

- Naive approach: Run one simple linear regression per feature. But! In this way the estimates ignore all other features left outside: Not always good, due to correlation among features.
- Correct approach: Extend the simple linear model to accommodate multiple predictors. Give to each predictor a separate slope coefficient in a single model,

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \epsilon. \tag{22}$$

Coefficient Estimation

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Again, the regression coefficients are unknown and must be estimated. We use the formula:

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \ldots + \hat{\beta}_k x_k. \tag{23}$$

We choose the parameters that minimise again the RSS

$$\begin{aligned} RSS &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i,1} - \hat{\beta}_2 x_{i,2} - \ldots - \hat{\beta}_k x_{i,k})^2 \end{aligned} \tag{24}$$

☞ Complicated expressions, better use existing software packages.

Least-squares plane

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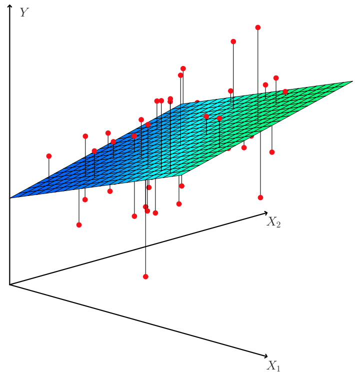

Figure: Regression plane for two features.[4]

[4] Source [B.1]

Hypothesis test (again)

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$$H_0 : \beta_1 = \beta_2 = \ldots = \beta_k = 0$$

versus

$$H_a : \text{ at least one } \beta_j \text{ non-zero.}$$

☞ To answer, we compute the *F-statistic*:

$$F = \frac{(TSS - RSS)/k}{RSS/(n-k-1)}, \tag{25}$$

$RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$, and $TSS = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the Total Sum of Squares.

If the *F-statistic* is very close to 1 then we expect no relationship between the response and the predictors. On the other hand, if H_a is true, we expect $F > 1$.

Variable selection

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How do we decide on the important variables that influence the y?
☞ use the F-statistic and the individual p-value.

- Use different combinations of features to derive the F-statistic. If for a specific combination among these the value of the statistic drops considerably, then this is an indicator that among the included features, some are unrelated to the response.
- From the individual p-values, the one with the highest p-value is a candidate to be removed from the model.
- The R^2 value determines how much of the data variance is explained by the model. If it is low then the feature set used does not contain much info.
- other selection methods (forward and backward selection...)

Potential Problems of Linear Regression

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- Non-linearity of the responce-predictor relationships.
- Correlation of error terms.
- Non-constant variance of error terms (heteroscedasticity)
- Outliers (e.g. incorrect data collection)
- High leverage points.

Use Residual plots to detect problems:
$(y_i - \hat{y}_i, x_i)$ or $(y_i - \hat{y}_i, \hat{y}_i)$.

Non-linearity

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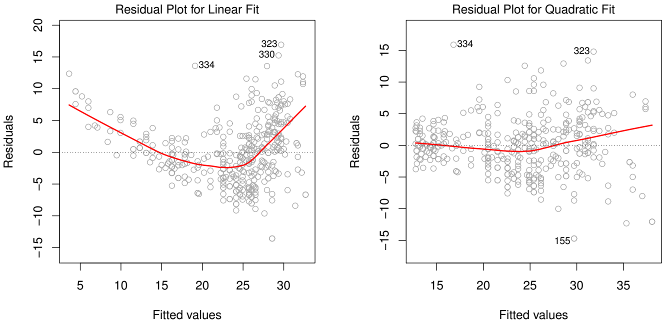

Figure: Residual plots for Linear and Polynomial fit.[5]

[5] Source [B.1]

Error Correlation

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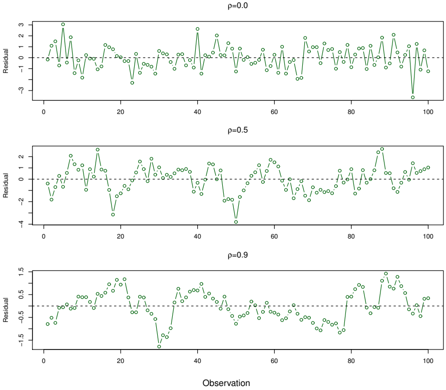

Figure: Residual plots for Time-series.[6]

[6] Source [B.1]

Heteroscedasticity

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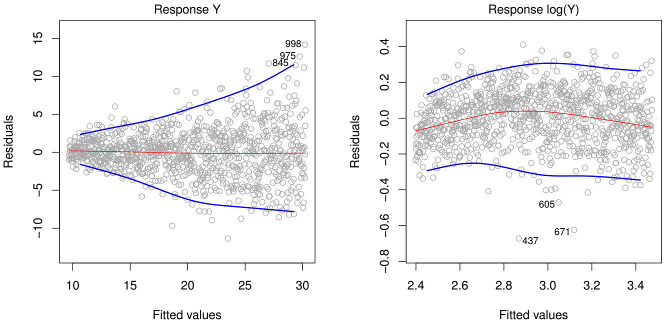

Figure: Residual plots for non-constant variance.[7]

[7] Source [B.1]

Outliers

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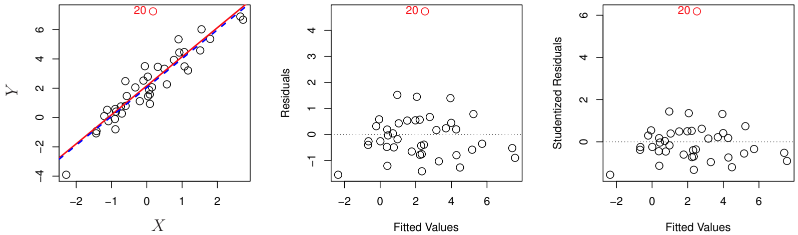

Figure: Effect of an outlier in least-squares fit.[8]

Outliers influences RSE, confidence intervals and p-values.

[8] Source [B.1]

High Leverage Points

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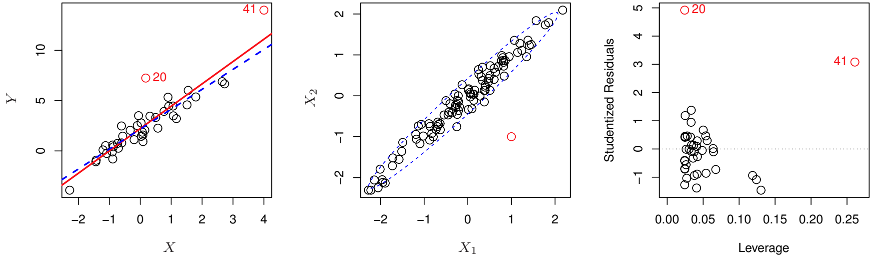

Figure: Effect of a high-leverage point in least-squares fit.[9]

[9] Source [B.1]

Collinearity

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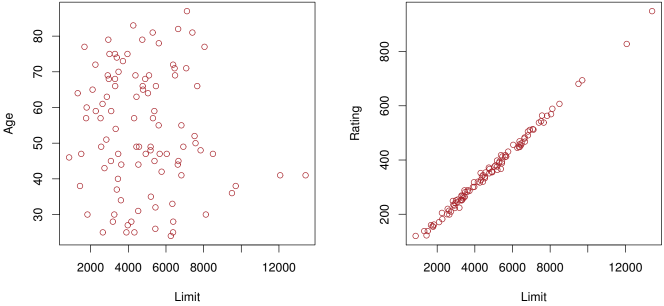

Figure: Effect of collinearity in least-squares fit.[10]

☞ Difficult to separate out the individual effects of collinear variables on the response.

[10] Source [B.1]

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END