# Diagnostics

UBCO MDS — DATA 570

# Potential Problems

- When we fit a linear regression model to a particular data set, a number of problems may occur.
- Today we will go through the most common among these.

# Non-linearity of the Data

The SLM assumes that the relationship between the predictors and the response fall ($\approx$) on a straight line.

When the true relationship deviates markedly from linear, then all conclusions/predictions derived from this fit are dubious at best.

# Non-linearity of the Data

Residual plots are a useful graphical tool for identifying non-linearity.

**SLR:** plot the residuals, $e_i = y_i - \hat{y}_i$, versus the predictor $x_i$.

**MLR:** plot the residuals versus the predicted (or fitted) values $\hat{y}_i$.

# Non-linearity of the Data

- Ideally, the residual plot will show no discernible pattern.
- The presence of a pattern may indicate a problem with some aspect of the linear model.
- A “good” plot should produce randomly dispersed residuals around the horizontal axis

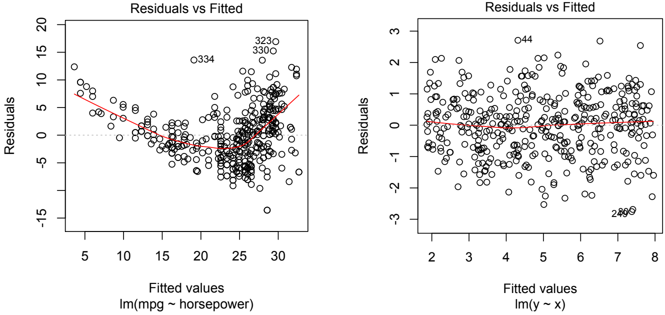



Figure: "Bad" (left) and "good" (right) residual plots.

# Residual Plots

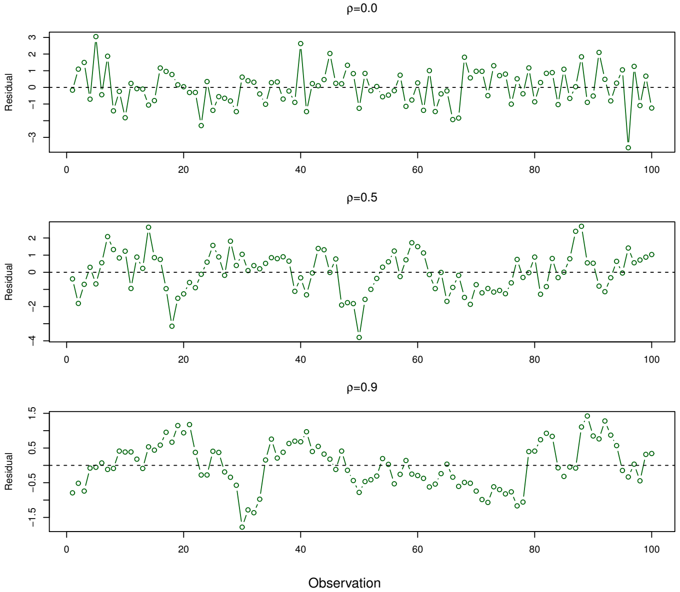
- To help us identify any trends, a red smooth line is fit to the residuals
- In the ideal scenario, this smooth line should be a horizontal line at 0.
- In presence of non-linear associations, we could try and fit a model with *transformed* predictors, eg. $\log(X)$, $\sqrt{X}$, and $X^2$, (as discussed in Lecture 5)

# Correlation of error terms

- As discussed in Lecture 2, the linear regression model assumes that the error terms, $e_1, e_2, \ldots, e_n$, are independent.
- If error terms are correlated, then the estimated standard errors will tend to underestimate the true standard errors.
- In other words, if the error terms are correlated, we may have an unwarranted sense of confidence in our model.

# Correlation of error terms

- Correlated errors can occur when multiple measurements are taken on the same subject over time (i.e *time series* data)
- To investigate this assumption violation, we plot the residuals from our model as a function of time.
- Other examples can be when our data contain
  - members of the same family
  - people exposed to the same environmental factors


ρ=0.0
ρ=0.5
ρ=0.9
Residual
Observation

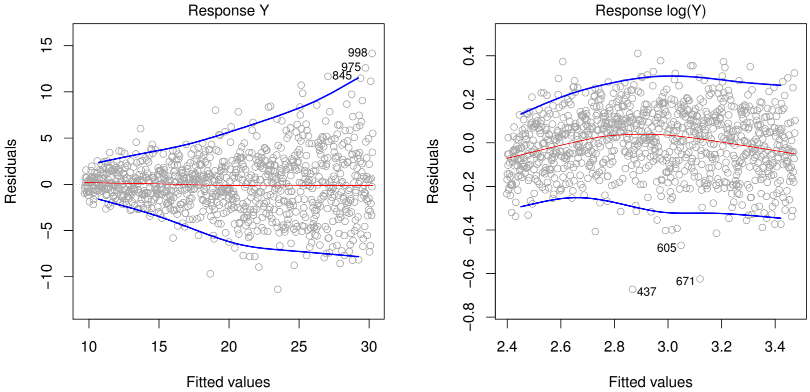
# Non-constant variance

- Non-constant variance of error terms, i.e. $Var(e_i) = \sigma^2$, is another important assumption of the linear regression model.

- This assumption is often violated, eg. the variances of the error terms may increase with the value of the response.

# Non-constant variance

- Non-constant variance, i.e. *heteroscedasticity* can be identified through the residual plot.
- Often this violation takes shape as a funnel/fan shape in the residual plot.
- In presence of non-constant variance, we could try transforming the *response* $Y$ using a concave function eg. $\log(Y)$, $\sqrt{Y}$.


Response Y
Residuals
Fitted values
998
975
845
Response log(Y)
Residuals
Fitted values
605
671
437

# Outliers

- An outlier is a point for which $y_i$ is far from the predicted value $\hat{y}_i$ (see next slide for example)

- Outliers can be genuine or be a result of, for example, incorrect reading/recording.

- If an outlier is believed to be a result of an error, then one might simply remove that observation.

- However, genuine outliers may indicate a deficiency with the model, eg. a missing predictor.

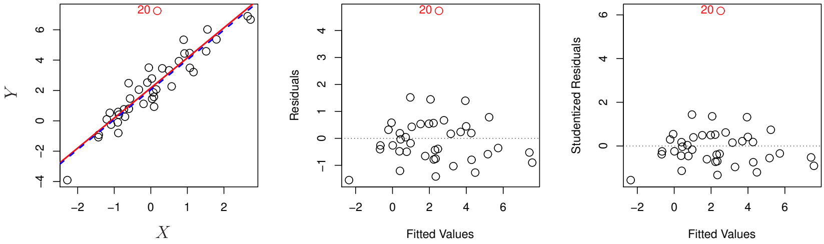



Figure: The red/blue line shows the fit with the outlier included/excluded.

# Outliers

- As depicted in the previous slide, it can happen that outliers do not greatly affect on the least squares regression line.

- It can however affect things like RSE, $p$-values, and $R^2$ values.

- Again, residual plots can be useful in identifying outliers.

# Outliers

- To avoid arbitrary cut-offs in a residual plot, sometimes we turn to the so-called *studentized residuals*
- These scaled residuals are produced by dividing each residual $e_i$ by its estimated standard studentized error, $se(e_i) = \sqrt{MSE(1 - h_i)}$
- Observations whose studentized residuals are greater than 3 are then flagged as potential outliers.

# High-leverage points

- While outliers produce unusual $y_i$ values, observations with high leverage have unusual $x_i$ values.
- The inclusion/exclusion of high leverage points tend to have a higher impact on estimated regression line
- It is very important to identify such points as they have the potential to invalidate the entire fit.

# High-leverage points

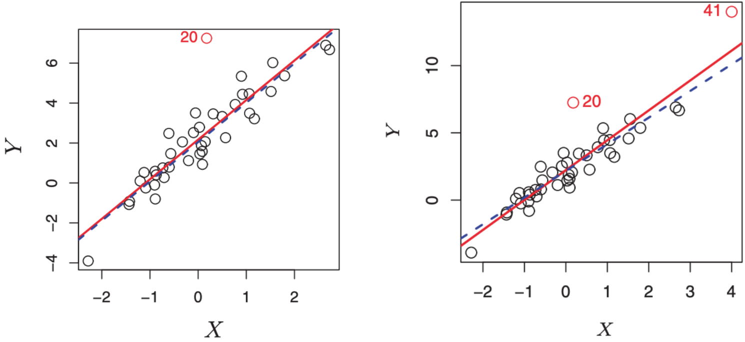



Figure: Left: example of outlier Right: example of high-leverage. The red (blue) line shows the fit with the outlier/high-leverage included (excluded)

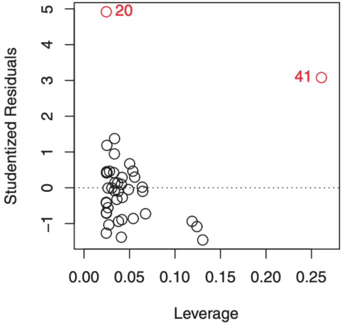
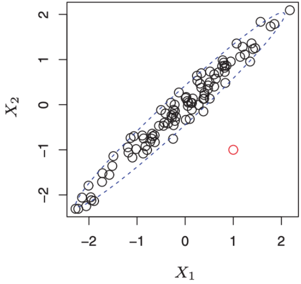



Figure: Plotting the studentized residuals versus $h_i$ flags observation 41 is an outlier as well as a high-leverage point, while observation 20 is an outlier with low leverage.

- For SLR high leverage can be easily identified by looking for observations having predicted values outside of the “normal” range

- With MLR, these points can be harder to identify.



High-leverage observations will have larger values of the so-called *leverage statistic*. For SLR:

$$h_i = \frac{1}{n} + \frac{x_i - \overline{x}}{\sum_j^n (x_j - \overline{x})^2} \tag{1}$$

As the distance between $x_i$ and $\overline{x}$ increase, so to does the $h_i$.

For MLR, leverage is given the *i*th diagonal element of the *hat* matrix:

$$H = X^T(X^T \cdot X)^{-1}X \tag{2}$$

In words: how far the vector $(X_{i1}, X_{i2} \ldots X_{ip})$ is from $(\overline{X}_1, \overline{X}_2 \ldots \overline{X}_p)$, with distance measured in standard deviation units.

A general guideline is to use $h_i > 2(p+1)/n$ as an indicator for high leverage (note: $1/n \leq h_i \leq 1$)

# Influential points

- Observations having a relatively large effect on the regression model's predictions are called influential observations
- A high leverage point is not necessarily an influential point.
- An influential point is not necessarily a high leverage point.

# Influential points

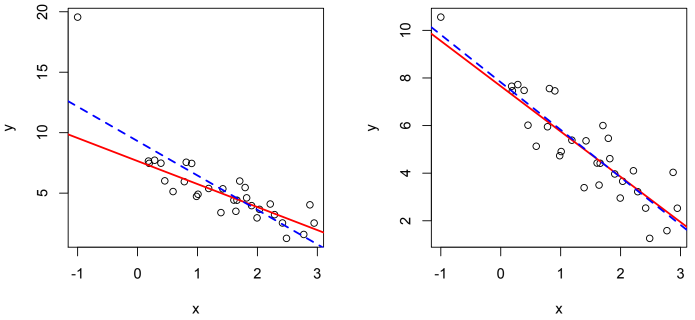



Figure: Left: Influential high leverage outlier Right: High leverage

# Influential points

- A typical measure of influence is the Cook's D-statistic.

- The Cook's distance statistics, for observation $i$:

$$D_i = \frac{e_i^2}{MSE \cdot d} \left[ \frac{h_i}{(1 - h_i)^2} \right] \tag{3}$$

where $d$ is the dimension of your data (ie. $X_{n \times d}$)

- Influential observations will have high Cook's distance score.

# Collinearity

- Collinearity occurs when two or more predictor variables are closely related to one another.
- Simple bivariate scatterplots can show us correlations between predictors
- However, one variable may be correlated with some *linear combination* of two or more other variables (multicollinearity)

# Collinearity

- Collinearity reduces the accuracy of the estimates of the regression coefficients, ie. increase $SE(\hat{\beta}_j)$.
- Consequently, the *power* of the hypothesis test—the probability of correctly power detecting a non-zero coefficient—is reduced by collinearity

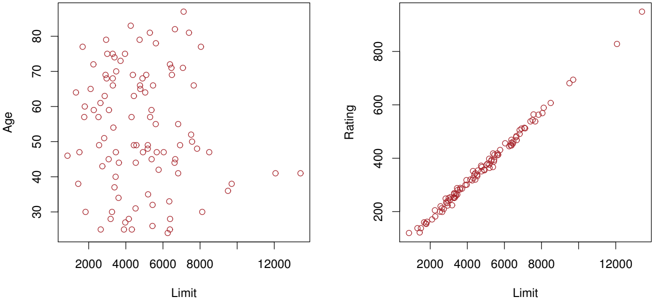



Figure: **ISLR Figure 3.14:** Scatterplots of the observations from the `Credit` data set. Left: A plot of `age` versus `limit`. These two variables are not collinear. Right: A plot of `rating` versus `limit`. There is high collinearity

| | | Coefficient | Std. error | t-statistic | p-value |
|---|---|---|---|---|---|
| | Intercept | −173.411 | 43.828 | −3.957 | < 0.0001 |
| Model 1 | age | −2.292 | 0.672 | −3.407 | 0.0007 |
| | limit | 0.173 | 0.005 | 34.496 | < 0.0001 |
| | Intercept | −377.537 | 45.254 | −8.343 | < 0.0001 |
| Model 2 | rating | 2.202 | 0.952 | 2.312 | 0.0213 |
| | limit | 0.025 | 0.064 | 0.384 | 0.7012 |

**TABLE 3.11.** *The results for two multiple regression models involving the* `Credit` *data set are shown. Model 1 is a regression of* `balance` *on* `age` *and* `limit`*, and Model 2 a regression of* `balance` *on* `rating` *and* `limit`*. The standard error of* $\hat{\beta}_{\text{limit}}$ *increases 12-fold in the second regression, due to collinearity.*

# Collinearity

- The most straightforward measure of collinearity is called the Variance Inflation Factor (VIF).
- VIF measures the ratio of the variance of $\hat{\beta}_j$ in the full model and the variance of $\hat{\beta}_j$ if it were fit on its own (i.e SLR).
- A VIF$=$1 (smallest possible value) indicates the complete absence of collinearity

# Collinearity

- The VIF is calculated as follows:

$$VIF(\hat{\beta}_j) = \frac{1}{1 - R_j^2}$$

  where $R_j^2$ is the $R^2$ for the regression of $X_j$ on all the other $X_s$.

- If $R_j^2$ is close to one, then collinearity is present, and so the VIF will be large.

- Typically values exceeding 10 indicate a problem.

# Collinearity

- In practice small amount of collinearity among the predictors is expected
- VIFs do not tell how many collinearities there are, or which variables are included in them.
- There are other more sophisticated measures of collinearity (eg. based on eigenvalues and eigenvectors of the matrix of $X$s) but those fall outside the scope of this module.

# Collinearity

In the face of collinearity, we may decide to:

- eliminate one of the problematic variables our model
- combine the collinear variables together into a single predictor

# Diagnostic Plots

If we apply the `plot()` function fo the output from a `lm()` (see `?plot.lm` for details), four diagnostic plots are produced:

1. Residuals vs Fitted
2. Normal Q-Q plot
3. Scale-Location
4. Residuals vs Leverage

# Normal Q-Q plot

- A normal Q-Q plot shows if residuals are normally distributed.
- More generally, a Q-Q (quantile-quantile) plot plots two sets of quantiles against one another.
- Quantiles coming from the same distribution should roughly form points along a straight line

# Normal Q-Q plot for normal data

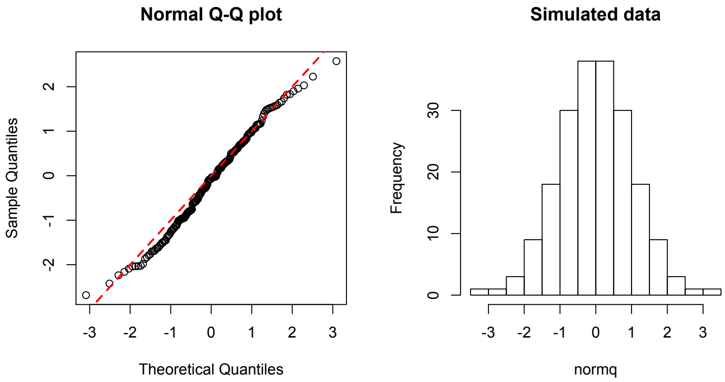



Figure: Normal data will tend to produce points on the dashed line of a Normal Q-Q plot.

# Normal Q-Q plot

- While visual checks of this sort are subjective, it allows us to see at-a-glance if our assumption is plausible, and if not, how the assumption is violated and what data points contribute to the violation.
- This is not a formal test unlike other statistical approaches
- If points fall very far from a straight line, that is cause for concern.

# Normal Q-Q plot for skewed data

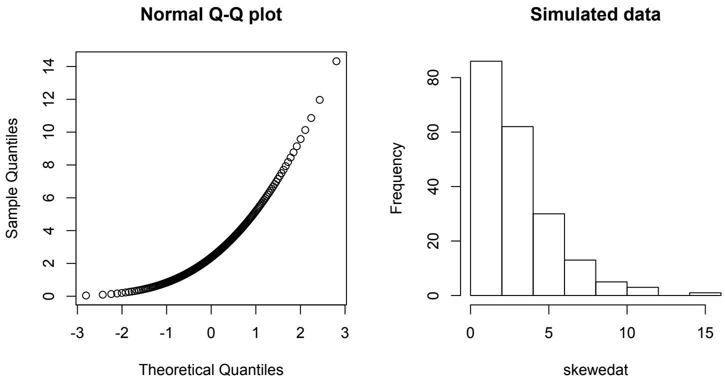



Figure: Curved Normal Q-Q plots may be an indication that your data are skewed.

# Normal Q-Q plot for heavy-tailed data

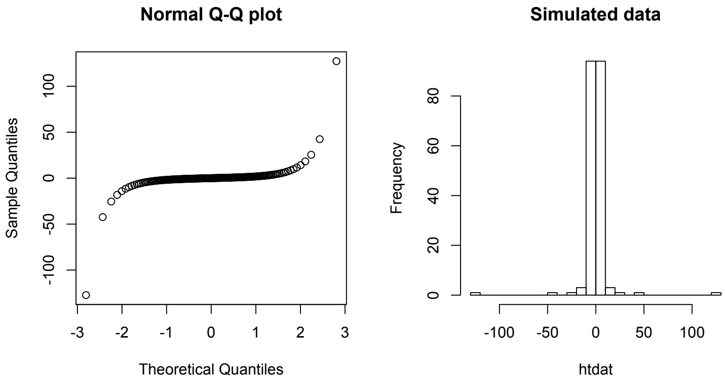



Figure: Normal Q-Q plots that are flat in the middle and highly curved at extremities may indicate heavy-tailed data.

# Conclusion

- While many of the steps towards fitting a linear regression model are algorithmic, model building is more an art than a science.
- These diagnostics tools are meant to guide you through making a decision, but the decision is ultimately yours.