Statistics 305/605: Introduction to Biostatistical Methods for Health Sciences

Chapter 18, part 3: Prediction intervals, r^2, residual plots

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Prediction Intervals (PIs)

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- $\hat{y} = \hat{\alpha} + \hat{\beta}x$ is also our prediction of a *future* y at x.
- Future y's consist of the population parameter $\mu_{y|x}$ **plus** a random error.
- The CI is an interval that estimates the parameter $\mu_{y|x}$.
- In contrast, a PI is an interval that predicts $\mu_{y|x}$ **plus** a random error and so should be wider (more variable) than the CI.
- To construct an interval that contains, say, 95% of all future y's, we need to account for 2 sources of variation:
  1. variation in $\hat{\mu}_{y|x} = \hat{\alpha} + \hat{\beta}x$, and
  2. variation in ϵ.
- As a result of the extra-variation due to ϵ in 2 above, over and above the variation in $\hat{\mu}_{y|x}$ in 1 accounted for by the CI, the PIs are wider than CIs.

- A level-C PI has the usual form of

$$\text{estimate} \pm \text{margin of error},$$

  where

  - the estimate is $\hat{y}$, and
  - the margin of error is $SE(\text{pred})$ times t^*, the upper $(1-C)/2$-critical value of the t-distribution with $n-2$ df.
- The PI is of similar form to the CI for $\mu_{y|x}$, except that $SE(\hat{y})$ is replaced with the larger **standard error of prediction**, $SE(\text{pred})$.
  - The text, page 430, provides the formula, which we'll skip. (Text's notation for $SE(\text{pred})$ is $\widehat{se}(\tilde{y})$).

95% CIs and PIs for example data

- Predicted values $\hat{y}$ and lower and upper limits of PI are in the columns `fit`, `lwr` and `upper`, respectively.
- PIs are wider than CIs; e.g. in the low birth-weight babies data ...

95% CI for the mean head circumference at gestational age 29 weeks is (26.22, 26.85) cm:

```
##   gestage      fit      lwr      upr
## 1      29 26.53581 26.21989 26.85172
```

95% PI for the head circumference at gestational age 29 weeks is (23.36, 29.71) cm:

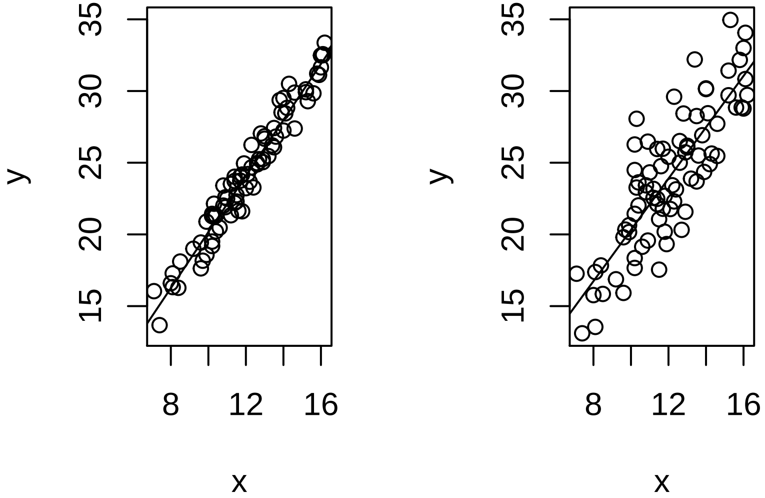
```
##   gestage      fit      lwr     upr
## 1      29 26.53581 23.36391 29.7077
```

r^2 in Simple Linear Regression

Coefficient of determination

- In simple line regression, the squared Pearson correlation, r^2, is called the *coefficient of determination*
- r^2 reflects how close the data are to the regression line.
- Specifically, r^2 is the fraction of the variation in the values of Y that is explained by the least-squares regression of y on x;
  - i.e. $r^2 = \text{explained variation}/\text{total variation}$.
- Examples:
  - if $r = 1$ or $r = -1$, $r^2 = 1$ and the regression explains 100% of the variation in y.
  - if $r = .7$ or $r = -.7$, $r^2 = .49$ and the regression explains 49% (about half) of the variation in y.

- Which of the two fitted models below do you think has a higher r^2 value?



- In the plot on the previous slide, the fitted line on the left accounts for 95% of the total variance in the responses, whereas the one on the right accounts for 70%.
- The more variance in the response that is accounted for by the regression model, the closer the data points will fall to the fitted regression line.
- If a model could explain 100% of the variance in y, the fitted values would be the observed values and all the data points would fall on the fitted line.

r^2 for low birth-weight babies

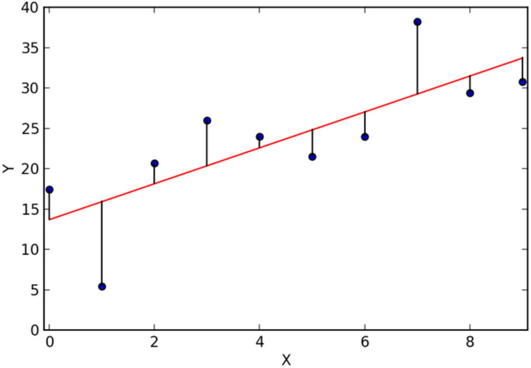
- In the low birth-weight babies example, the coefficient of determination for the regression of head circumference on gestational age is $r^2 \approx 0.61$ (see demo)

```
## [1] 0.6094799
```

Residual Plots

Residual plots

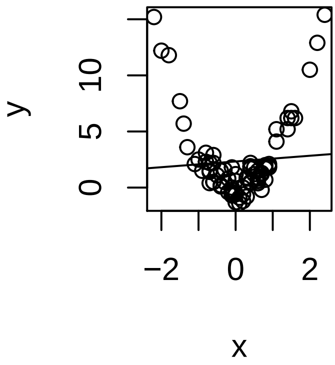
- Regardless of the coefficient of determination, we should look at the residuals to see what the data suggest about the adequacy of our regression model.
- Residuals are the discrepancies $y - \hat{y}$; i.e., the vertical distances between the observed values and the fitted values.
  - They are the primary tool for checking model assumptions.

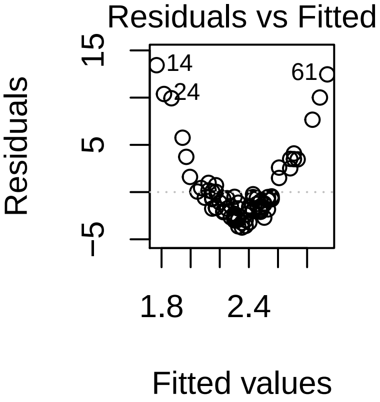


- We'll study regression diagnostics later in the course. For now, we only consider the plot of residuals vs. fitted values.
- This plot can show evidence of
  1. departures from the assumption of a linear relationship:
     - look for nonlinear trends
  2. departures from the assumption of constant SD
     - look for funnel shapes (e.g., text, page 435, Figure 18.11)
  3. departures from the assumption of no outlying/unusual data points:
     - look for unusually large residuals

Departures from linearity: EG.1

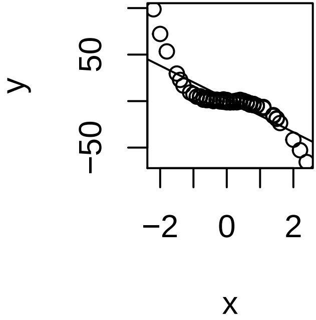
- Scatterplots of
  - (left) y vs. x with fitted regression line superposed, and
  - (right) residuals vs. $\hat{y}$.
- Both show that an obvious quadratic trend is missed by the fitted regression line.

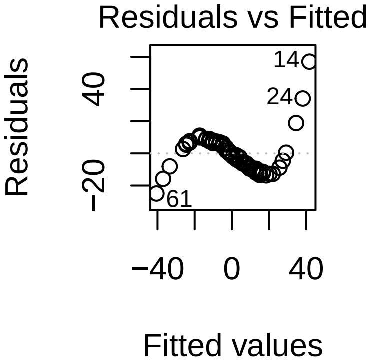




Departures from linearity: EG.2

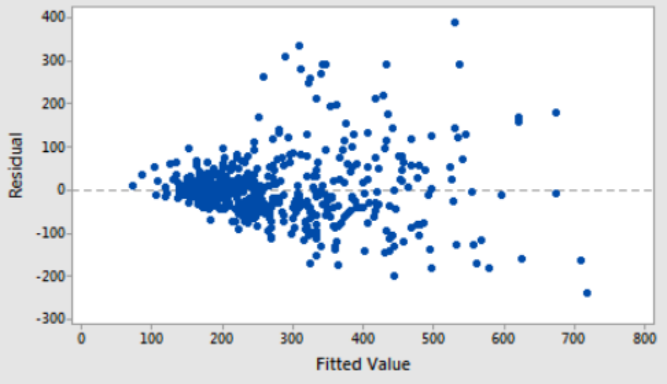
- Scatterplots of
  - (left) y vs. x with fitted regression line superposed, and
  - (right) residuals vs. $\hat{y}$.
- Both show that a nonlinear trend is missed by the fitted regression line, but it is more obvious in the plot of the residuals vs. fitted values on the right.





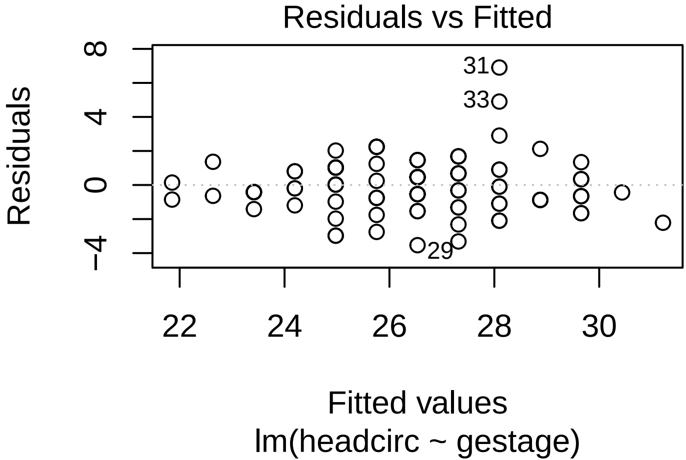
Departures from constant SD

- We can also use the plot of residuals vs. $\hat{y}$'s to look for non-constant SD in the response over the values of x
- Plot below suggests non-constant SD.
  - The funnel shape indicates that as $\hat{y}$ increases so does the spread of the residuals;
  - Suggests that, as population mean response increases, so does the response sd.



Outliers

- Finally, the plot of the residuals vs $\hat{y}$'s can help to find outliers.
- Let's look at the regression of head circumference on gestational age in the low-birthweight-babies data …



Interpretation

- There may be a few outliers among the observations such as infants 29, 31 and 33.
    - Infant 29 has a head circumference that is smaller than expected given his/her gestational age (negative residual)
    - Infants 31 and 33 have head circumferences that are larger than expected given their gestational age (positive residuals).
- However, there is no obvious non-linear trend that we've missed and no funnel shapes in the pattern of residuals.