Diagnostics

- Internally studentized residuals, PRESS residuals or externally studentized (case-deleted) residuals.
- Leverage.
- An individual point have large impact on $\hat{\mu}_i$. Diagnostic tool: DFFITS.
- An individual point may have large impact on $\hat{\mu}$ (the whole vector). Diagnostic tool: Cook’s distance.
- An individual point may have large impact on $\hat{\beta}$. Diagnostic tool: DFBETAS.
- Modified Levene test for heteroscedasticity; see text.
- Breusch-Pagan test for heteroscedasticity; see text.
- Shapiro Wilk test for normality.
- Added variable plot.
- Pure error sum of squares $F$ test.
Leverage

- Leverage $i$ is $h_{ii}$ — diagonal entry in hat matrix, $H$.
- $\text{Var}(\hat{\mu}_i) = h_{ii}$ and $\text{Var}(\hat{\epsilon}_i) = 1 - h_{ii}$ so $0 \leq h_{ii} \leq 1$.
- $\text{trace}(H) = p$ so the $h_{ii}$ average to $p/n$.
- Rule of thumb. $h_{ii} > 2p/n$ is “large” leverage.
- Rule of thumb. $h_{ii} > 0.5$ is large, $h_{ii} > 0.2$ is moderately large.
DFFITS

Measure change in fitted value for case $i$ after deleting case $i$:

$$(DFFITS)_i = \frac{\hat{Y}_i - \hat{Y}_{i(i)}}{\sqrt{\text{MSE}(i)h_{ii}}}$$

- Any subscript $(i)$ refers to a computation with case $i$ deleted.
- Can be computed from externally deleted residual by multiplying by $\sqrt{h_{ii}/(1 - h_{ii})}$. Thus can be computed without actually deleting case $i$ and rerunning.
- Rule of thumb from text: look out for $|DFFITS| > 1$ in small to medium data sets or for $|DFFITS| > 2\sqrt{p/n}$ in large data sets.
- But I just examine the few largest values.
Cook’s Distance

An individual point may have large impact on \( \hat{\mu} \) (the whole vector):

\[
D_i = \frac{\sum_{j=1}^{n}(\hat{Y}_j - \hat{Y}_{j(i)})^2}{p\text{MSE}}
\]

- Can be computed without deleting case from

\[
D_i = \frac{\hat{\epsilon}_i^2}{p\text{MSE}} \left[ \frac{h_{ii}}{(1 - h_{ii})^2} \right]
\]

- To judge size compare to \( F_{p,n-p,0.90} \) (lower tail area is 10%, usually found as 1 over upper 10% point of \( F_{n-p,p} \)) and to \( \text{median}(F_{p,n-p}) \).

- Bigger than latter is quite serious.

- Smaller than former is good.

- Between is gray zone.
DFBETAS

- Intended to measure impact of deleting case $i$ on $\hat{\beta}_k$.
- Defined by:

$$DFBETAS_{k(i)} = \frac{\hat{\beta}_k - \hat{\beta}_{k(i)}}{\sqrt{MSE(i) \left[ (X^T X)^{-1} \right]_{kk}}}$$

- Same guidelines as DFFITS.
- Software not always set up to compute DFBETAS.
Tests for Homoscedasticity

- **Modified Levene test:**
  - Split data set into 2 parts on basis of covariates
  - Fit regressions in each part separately.
  - Do 2 sample $t$-test on mean absolute size of residuals.

- **Breusch-Pagan test:**
  - Regress squared fitted residual on covariate or covariates
  - Test for non-zero slope.
Tests of Distributional Assumptions

- Check assumption of Normality.
- Examine $Q - Q$ plot for straightness.
- Shapiro-Wilk test applied to residuals
- Or correlation test in Q-Q plot.
Pure Error Sum of Squares

- Sometimes for each (or at least sufficiently many) combination of covariates in a data set, there are several observations.
- Can do extra sum of squares $F$-test to see if our regression model is adequate.
- Suppose that $x_1, \ldots, x_K$ are the distinct rows of the design matrix.
- Suppose we have $n_1$ observations for which the covariate values are those in $x_1$, $n_2$ observations with covariate pattern $x_2$ and so on. Of course $n_1 + \cdots + n_K = n$.
- We compare our final fitted model with a so-called saturated model by an extra sum of squares $F$-test.
- To be precise let $\alpha_1$ be the mean value of $Y$ when the covariate pattern is $x_1$, $\alpha_2$ the mean corresponding to $x_2$ and so on.
- Relabel the $n$ data points as $Y_{i,j}; j = \ldots, n_i; i = 1, \ldots, K$
- Fit a one way ANOVA model to the $Y_{i,j}$. 
Pure Error Sum of Squares

- Error sum of squares for this FULL model is

\[ ESS_{FULL} = \sum_{i=1}^{K} \sum_{j=1}^{n_i} (Y_{i,j} - \bar{Y}_{i,.})^2 \]

- This ESS is called the pure error sum of squares because we have not assumed any particular relation between the mean of \( Y \) and the covariate vector \( x \).

- We form the \( F \) statistic for testing the overall quality of our model by computing the “lack of fit SS” as

\[ ESS_{Restricted} - ESS_{FULL} \]

where the restricted model is the final model whose fit we are checking.
### Example: plaster hardness

- 9 different covariate patterns: 3 levels of SAND and 3 levels of FIBRE.
- Two ways to compute pure error sum of squares:
  - Create new variable with 9 levels.
  - Fit a two way ANOVA with interactions.

```plaintext
DATA

<table>
<thead>
<tr>
<th>0</th>
<th>0</th>
<th>1</th>
<th>61</th>
<th>34</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>63</td>
<td>16</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>2</td>
<td>67</td>
<td>36</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>2</td>
<td>69</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>50</td>
<td>9</td>
<td>74</td>
<td>48</td>
</tr>
</tbody>
</table>
```
data plaster;
infile 'plaster1.dat';
input sand fibre combin hardness strength;
proc glm data=plaster;
  model hardness = sand fibre;
run;
proc glm data=plaster;
  class sand fibre;
  model hardness = sand | fibre;
run;
proc glm data=plaster;
  class combin;
  model hardness = combin;
run;
**EDITED OUTPUT**

Complete output

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>Squares</th>
<th>Mean Square</th>
<th>F</th>
<th>Pr &gt; F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>2</td>
<td>167.41666667</td>
<td>83.70833333</td>
<td>11.53</td>
<td>0.0009</td>
</tr>
<tr>
<td>Error</td>
<td>15</td>
<td>108.86111111</td>
<td>7.25740741</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>17</td>
<td>276.27777778</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>Squares</th>
<th>Mean Square</th>
<th>F</th>
<th>Pr &gt; F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>8</td>
<td>202.77777778</td>
<td>25.34722222</td>
<td>3.10</td>
<td>0.0557</td>
</tr>
<tr>
<td>Error</td>
<td>9</td>
<td>73.50000000</td>
<td>8.16666667</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>17</td>
<td>276.27777778</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
From the output we can put together a summary ANOVA table:

<table>
<thead>
<tr>
<th>Source</th>
<th>df</th>
<th>SS</th>
<th>MS</th>
<th>F</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>2</td>
<td>167.417</td>
<td>83.708</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lack of Fit</td>
<td>6</td>
<td>35.361</td>
<td>5.894</td>
<td>0.722</td>
<td>0.64</td>
</tr>
<tr>
<td>Pure Error</td>
<td>9</td>
<td>73.500</td>
<td>8.167</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total (Corrected)</td>
<td>17</td>
<td>276.278</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- $F$ statistic is 
  \[ ((108.86111111 - 73.50000000)/6)/[8.16666667]. \]
- $P$-value comes from the $F_{6,9}$ distribution.
- $P$-value not significant: no reason to reject final fitted model which was additive and linear in each of SAND and FIBRE.
- Notice that the Error SS are the same for the two-way ANOVA with interactions, which is the second model, and for the 1 way ANOVA.
This test is not very powerful in general.

More sensitive tests are available if you know how the model might break down.

For instance, most realistic alternatives will be picked up more easily by checking for quadratic terms in a bivariate polynomial model; see earlier lectures.

Notice that test for any effect of SAND and FIBRE carried out in the one way analysis of variance is not significant.

This is an example of the lack of power found in many $F$-tests with large numbers of degrees of freedom in the numerator.

If you can guess a reasonable functional form for the effect of the factors (either the additive two way model with no interactions or the even simpler multiple regression model which is the first model above) you will get a more sensitive test usually.
Added Variable Plots or partial regression plots

- Regress $Y$ on some covariates $X_1$.
- Get Residuals.
- Regress other covariate $X_2$ on $X_1$.
- Get Residuals.
- Plot two sets of residuals against each other.
SENIC data example

Fit final selected model: covariates used are STAY, CULTURE, NURSES, NURSE.RATIO.

```sas
options pagesize=60 linesize=80;
data scenic;
  infile 'scenic.dat' firstobs=2;
input Stay Age Risk Culture Chest Beds School Region Census Nurses Facil;
   Nratio = Nurses / Census ;
proc glm data=scenic;
  model Risk = Culture Stay Nurses Nratio ;
  output out=scout P=Fitted PRESS=PRESS H=HAT RSTUDENT=EXTST R=RESID DFFITS=DFFITS COOKD=COOKD;
run ;
proc print data=scout;
```

Complete SAS Output is here.
Index plot of leverages

Outlying X Values

Observation Number

Leverage

0 20 40 60 80 100

0.0 0.05 0.10 0.15 0.20 0.25 0.30

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Index plot of leverages: discussion

- Observations 4, 8, 47, 54 and 112 have leverages over 0.15.
- Many more are over 10/113 — the suggested cut off.
- I prefer to plot the leverages and look at the largest few.
- Observations 4 and 47, in particular, have leverages over 0.3 and should be looked at.
- That means scientist thinks about those hospitals!
Influence measures: Cook’s Distance

Influence on entire fitted vector

Observation Number

Cook's Distance
0 20 40 60 ... ···
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·
·
···
··
··
·
·
·
·
···
·
·
8
11
54 112

Richard Lockhart
STAT 350: Diagnostics
Cook’s distance: discussion

- Observations 8, 11, 54 and 112 have values of $D_i$ larger than 0.05.
- Of these, only observation 11 is new.
- Text recommends worrying only about observations for which $D_i$ is larger than the tenth to twentieth percentile of the $F_{p,n-p}$ distribution.
- In this case those critical points are 0.3? and 0.46.
- None of the observations exceeds even the lowest of these numbers.
Influence measures: DFFITS

Influence on fitted values

Observation Number

DFFITS

0 20 40 60 80 100

-1.0 -0.5 0.0 0.5
Case deleted residuals

Externally Studentized Residuals

Observation Number

Residual

0 20 40 60 80 100

-2 -1 0 1 2
Case deleted residuals: discussion

- Only observation 53 is added for our consideration,
- But with 113 residuals a value of 2.9 is not terribly unusual.
Examine observations highlighted by diagnostics

Here are the covariate values for observations 4, 8, 11, 47, 53, 54 and 112:

<table>
<thead>
<tr>
<th>Observation</th>
<th>Culture</th>
<th>Stay</th>
<th>Nurses</th>
<th>Nratio</th>
<th>Risk</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>18.9</td>
<td>8.95</td>
<td>148</td>
<td>2.79</td>
<td>5.6</td>
</tr>
<tr>
<td>8</td>
<td>60.5</td>
<td>11.18</td>
<td>360</td>
<td>0.90</td>
<td>5.4</td>
</tr>
<tr>
<td>11</td>
<td>28.5</td>
<td>11.07</td>
<td>656</td>
<td>1.11</td>
<td>4.9</td>
</tr>
<tr>
<td>47</td>
<td>17.2</td>
<td>19.56</td>
<td>172</td>
<td>0.63</td>
<td>6.5</td>
</tr>
<tr>
<td>53</td>
<td>16.6</td>
<td>11.41</td>
<td>273</td>
<td>0.83</td>
<td>7.6</td>
</tr>
<tr>
<td>54</td>
<td>52.4</td>
<td>12.07</td>
<td>76</td>
<td>0.66</td>
<td>7.8</td>
</tr>
<tr>
<td>112</td>
<td>26.4</td>
<td>17.94</td>
<td>407</td>
<td>0.51</td>
<td>5.9</td>
</tr>
<tr>
<td>Mean</td>
<td>15.8</td>
<td>9.65</td>
<td>173</td>
<td>0.95</td>
<td></td>
</tr>
<tr>
<td>SD</td>
<td>10.2</td>
<td>1.91</td>
<td>139</td>
<td>0.11</td>
<td></td>
</tr>
</tbody>
</table>
Observation 4 has a quite unusual value of Nurse.Ratio – a lot of nurses.

Observation 47 has quite a high average Stay for patients.

The others are harder to interpret but 4 and 47 are the most leveraged observations.

In summary it appears that several observations exert excess influence on the fitting process.

As a final method of judging whether or not our fit was unduly influenced by these observations I fit the model again in SAS but removing observations number 4, 8, and 47.
### Sum of Mean

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>Squares</th>
<th>Square</th>
<th>F</th>
<th>Pr &gt; F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>4</td>
<td>100.4617</td>
<td>25.1154</td>
<td>28.21</td>
<td>0.0001</td>
</tr>
<tr>
<td>Error</td>
<td>105</td>
<td>93.4950</td>
<td>0.8904</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>109</td>
<td>193.9567</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>R-Square</th>
<th>C.V.</th>
<th>Root MSE</th>
<th>RISK Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.517959</td>
<td>21.8708</td>
<td>0.9436255</td>
<td>4.3145455</td>
</tr>
</tbody>
</table>

### T for H0: Pr > |T| SE

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Est</th>
<th>Par=0</th>
<th>Est</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTERCEPT</td>
<td>-.15118</td>
<td>-0.21</td>
<td>0.8349 0.7237</td>
</tr>
<tr>
<td>CULTURE</td>
<td>0.05686</td>
<td>5.28</td>
<td>0.0001 0.0108</td>
</tr>
<tr>
<td>STAY</td>
<td>0.27735</td>
<td>4.18</td>
<td>0.0001 0.0663</td>
</tr>
<tr>
<td>NURSES</td>
<td>0.00167</td>
<td>2.30</td>
<td>0.0232 0.0007</td>
</tr>
<tr>
<td>NRATIO</td>
<td>0.70245</td>
<td>1.92</td>
<td>0.0578 0.3661</td>
</tr>
</tbody>
</table>

Compare these results to the corresponding parts of the same code applied to the full data set.
Dependent Variable: RISK

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>Squares</th>
<th>Square</th>
<th>F</th>
<th>Pr &gt; F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>4</td>
<td>103.6905</td>
<td>25.9226</td>
<td>28.66</td>
<td>0.0001</td>
</tr>
<tr>
<td>Error</td>
<td>108</td>
<td>97.6893</td>
<td>0.9045</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>112</td>
<td>201.3798</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

R-Square  C.V.  Root MSE  RISK Mean
0.514900  21.83920  0.9510681  4.3548673

T for H0: Pr > |T|  SE

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Estimate</th>
<th>Par=0</th>
<th>of Est</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTERCEPT</td>
<td>-.083138</td>
<td>-0.14</td>
<td>0.8917</td>
</tr>
<tr>
<td>CULTURE</td>
<td>0.048249</td>
<td>5.03</td>
<td>0.0001</td>
</tr>
<tr>
<td>STAY</td>
<td>0.276744</td>
<td>5.04</td>
<td>0.0001</td>
</tr>
<tr>
<td>NURSES</td>
<td>0.001587</td>
<td>2.26</td>
<td>0.0258</td>
</tr>
<tr>
<td>NRATIO</td>
<td>0.769487</td>
<td>2.57</td>
<td>0.0115</td>
</tr>
</tbody>
</table>

Summary: differences seem minor; little harm in sticking to model fitted earlier.
Making an Added variable plot: example

- For SENIC data to assess influence of facilities.
- Regress RISK on STAY, CULTURE, NURSES, NURSE.RATIO. Get residuals.
- Regress FACILITIES on STAY, CULTURE, NURSES, NURSE.RATIO. Get residuals.
- Plot residuals against each other. Look for patterns.
Added Variable Plot for FACILITIES

Residuals from Risk

Residuals from Facilities