Model Diagnostics

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Regression Analysis

Diagnostics we have already discussed

- Residuals e_i vs.
  - i (independence)
  - $x_1, \ldots, x_k$ (linearity)
  - $\hat{Y}_i$ (linearity and homogeneity of variance)

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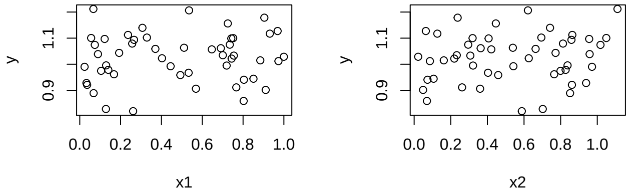
- Now we'll discuss
  - added variable plots,
  - leverages,
  - DFFITS,
  - Cook's distance.

The problem with marginal plots



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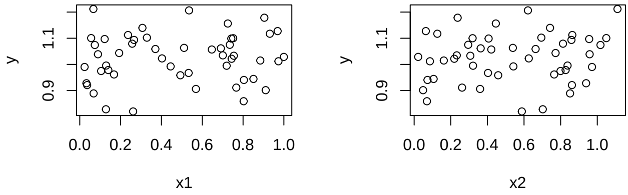

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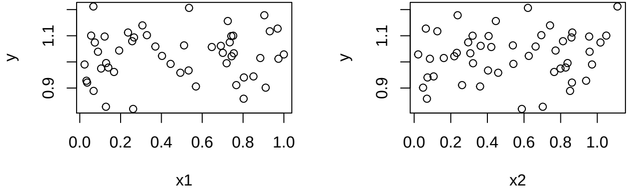

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x1           0.95536    0.07651  12.487   <2e-16 ***
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Added variable plots

Outliers, leverages, DFFITs, Cook's distance

Review of Diagnostics

Example

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- Residuals e_i versus a predictor values x_i, j can show whether x_j may need to be transformed or whether we should add a quadratic term x_j^2.

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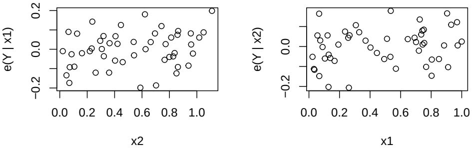

where $e(Y \mid x_j)$ are residuals when we regress Y on x_j only.

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- It answers the question: Does x_j explain any *residual* variability once the rest of the predictors are in the model?

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- If you fit a simple linear regression

$$e_i(Y \mid \mathbf{x}_{-j}) = \beta_j \cdot e_i(x_j \mid \mathbf{x}_{-j}) + \epsilon_i$$

then the LSE $\hat{\beta}_j$ *is the same* as one would get from fitting the full model $Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_k x_{ik} + \epsilon_i$.

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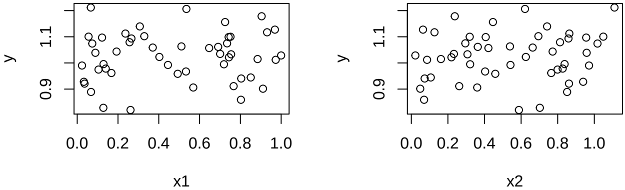
- Gives an idea of the functional form of x_j: a transformation in x_j should mimic the pattern seen in the plot.

10.1 Added variables plots illustration

Let's go back to our synthetic example:



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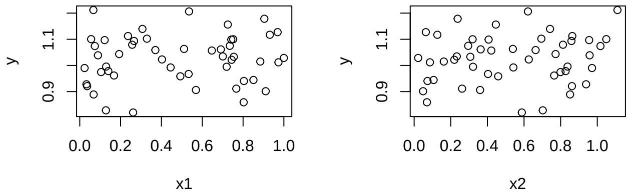

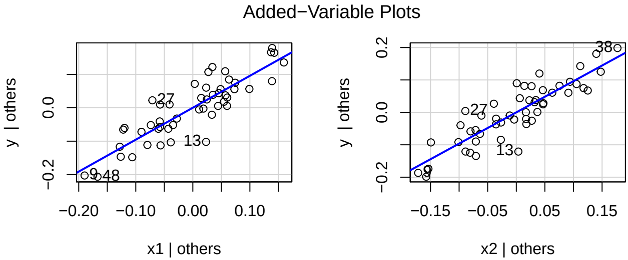

Salary data, first order terms only

```
> head(salary_data)
  salary age educ pol
1     38  25    4   D
2     45  27    4   R
3     28  26    4   O
4     55  39    4   D
5     74  42    4   R
6     43  41    4   O
> m = lm(salary ~ ., data=salary_data)
> summary(m)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  17.0313     7.3459   2.318  0.03735 *
age           0.8983     0.1968   4.565  0.00053 ***
educ          1.5039     1.1841   1.270  0.22632
polO        -16.5404     4.8807  -3.389  0.00484 **
polR          9.1587     4.8482   1.889  0.08139 .
---

Residual standard error: 8.209 on 13 degrees of freedom
Multiple R-squared:  0.8374,Adjusted R-squared:  0.7873
```

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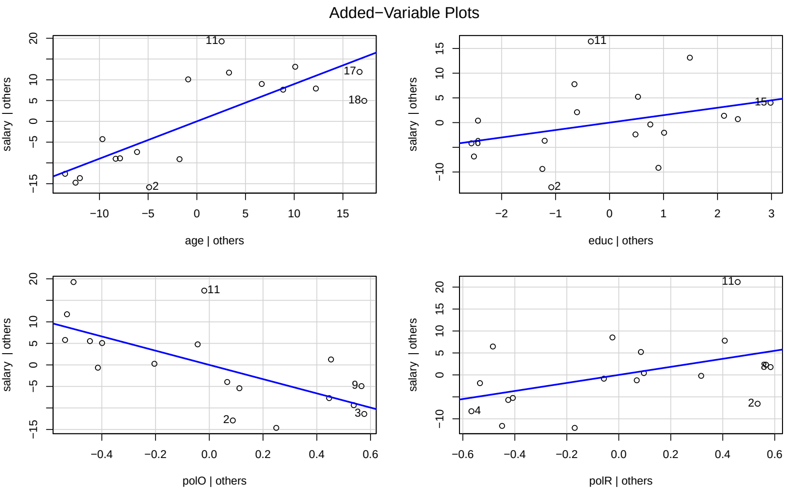

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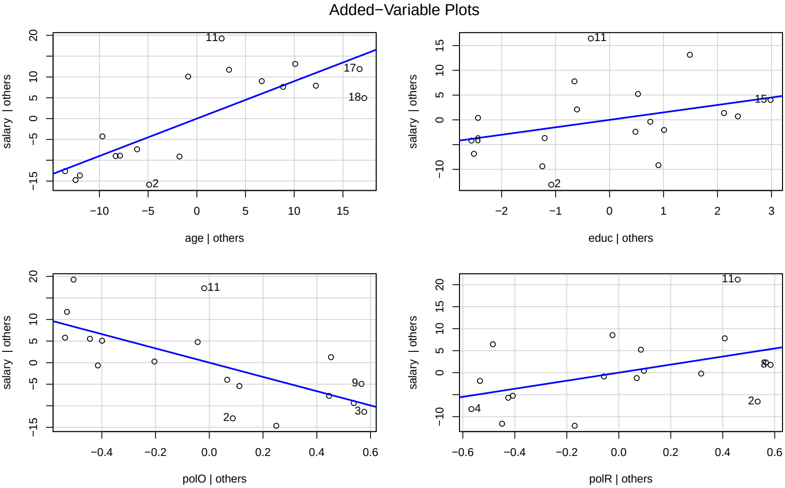


Age effect is nonlinear; let's add a quadratic term.

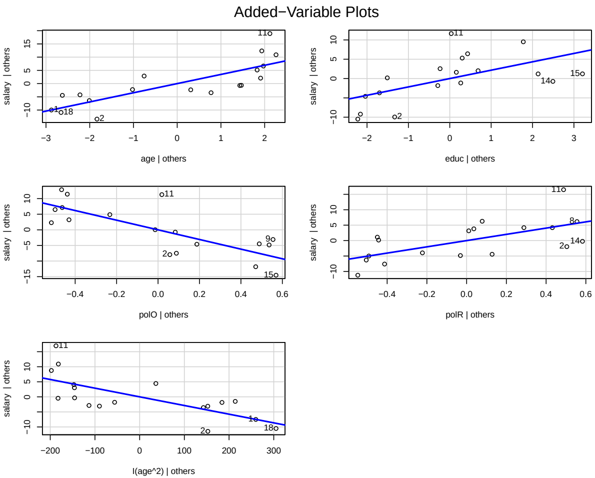
Salary data, quadratic effect in age

```
> m1 = lm(salary ~ . + I(age^2), data=salary_data)
> summary(m1)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -39.224169  16.810142  -2.333 0.037839 *
age           3.463723   0.740666   4.676 0.000535 ***
educ          2.166475   0.883369   2.453 0.030453 *
polO        -15.455108   3.571147  -4.328 0.000983 ***
polR         10.118144   3.544586   2.855 0.014500 *
I(age^2)     -0.028831   0.008166  -3.530 0.004143 **
---

Residual standard error: 5.984 on 12 degrees of freedom
Multiple R-squared:  0.9202,Adjusted R-squared:  0.887
```

Added variables plots w/ quadratic age



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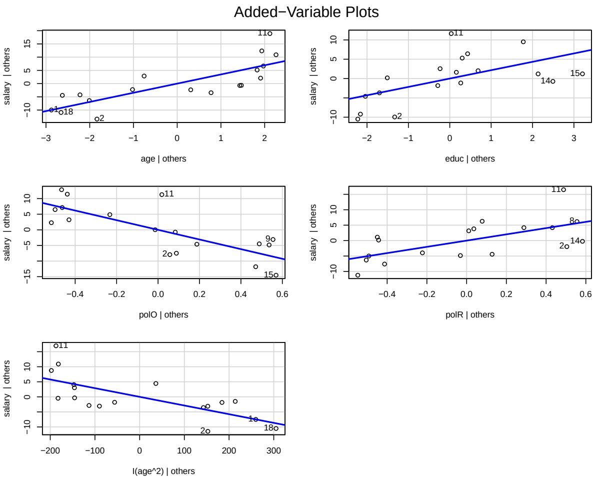


Education is now significant! The incorrect functional form for age was *masking* the importance of education.

Salary data, quadratic effect in education

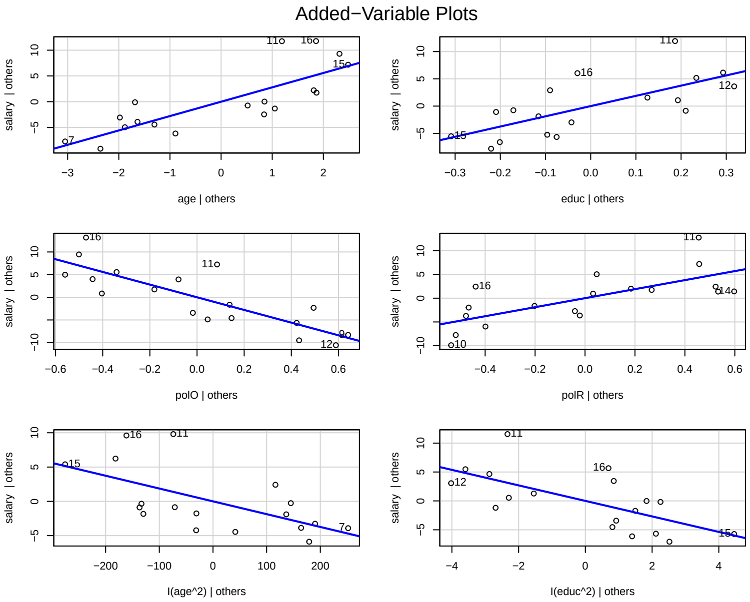
```
> summary(m2)

Call:
lm(formula = salary ~ . + I(age^2) + I(educ^2), data = salary_data)

              Estimate Std. Error t value Pr(>|t|)
(Intercept) -75.977348  18.262402  -4.160 0.001589 **
age           2.787032   0.626151   4.451 0.000977 ***
educ         18.751324   5.739109   3.267 0.007501 **
polD        -13.976910   2.848879  -4.906 0.000467 ***
polR          9.495127   2.790631   3.403 0.005903 **
I(age^2)     -0.018677   0.007298  -2.559 0.026558 *
I(educ^2)    -1.342341   0.461108  -2.911 0.014161 *
---

Residual standard error: 4.697 on 11 degrees of freedom
Multiple R-squared:  0.9549,Adjusted R-squared:  0.9304
```

Added variable plots w/ quad. age and educ



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  - if not, outlying values may skew inference a lot and yield models with poor predictive properties.

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- A **DFFIT** is a measure of influence that an individual point $(\mathbf{x}_i, Y_i)$ has on the regression surface at $\mathbf{x}_i$.
- **Cook's distance** is a consolidated measure of influence the point $(\mathbf{x}_i, Y_i)$ has on the regression surface at all n points $\mathbf{x}_1, \ldots, \mathbf{x}_n$.

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&= \sigma^2\mathbf{H}
\end{aligned}$$

$\Rightarrow \quad \mathrm{Var}[\hat{Y}_i] = \sigma^2 h_{ii}$, and its unbiased estimator is $\mathrm{MSE} \cdot h_{ii}$.

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- Typically, $|r_i| > 2$ is considered "large."
- $h_{ii} = \mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i$ is called the i^{th} **leverage value**.

10.2 Studentized deleted residuals

- The **standardized residuals**

$$r_i = \frac{Y_i - \hat{Y}_i}{\sqrt{\mathrm{MSE}(1 - h_{ii})}}$$

  have a constant variance of 1.
- Typically, $|r_i| > 2$ is considered "large."
- $h_{ii} = \mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i$ is called the i^{th} **leverage value**.
- A refinement of the standardized residual that has a recognizable distribution is the **studentized deleted residual**

$$t_i = \frac{Y_i - \hat{Y}_i}{\sqrt{\mathrm{MSE}_{(i)}(1 - h_{ii})}}$$

  where $\mathrm{MSE}_{i(i)}$ is obtained from the model when i-th example was removed from the data.

Studentized deleted residuals

- In fact, no need to fit n additional regressions, because there is relationship b/w MSE and $\text{MSE}_{(i)}$:

$$(n-p)\text{MSE} = (n-p-1)\text{MSE}_{(i)} + \frac{e_i^2}{1-h_{ii}}$$

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as outlying.
- Typically, in practice, one simply flags observations with $|t_i| > t_{1-\alpha/2;n-p-1}$ as *possibly* outlying in consideration with other diagnostics.

10.3 Leverage

- The leverages h_{ii} get larger the further the points $\mathbf{x}_i$ are from the mean $\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$, adjusted for "how many" other predictors are in the vicinity of $\mathbf{x}_i$.

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- Use the fact that $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top = \mathbf{H}\mathbf{H}$ to show $\sum_{i=1}^{n} h_{ii} = p$ and $0 \leq h_{ii} \leq 1$.

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- The rule of thumb is that any leverage h_{ii} that is larger than twice the mean leverage p/n, i.e. $h_{ii} > 2p/n$, is flagged as having "high" leverage.

Leverage

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- In `R`, you can get leverages using `hatvalues` command.

10.4 DFFITs

- The i^{th} DFFIT, denoted DFFIT_i, is given by

$$\text{DFFIT}_i = \frac{\hat{Y}_i - \hat{Y}_{i(i)}}{\sqrt{\text{MSE}_{(i)} h_{ii}}} = t_i \sqrt{\frac{h_{ii}}{1 - h_{ii}}},$$

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- Rule of thumb that DFFIT_i is "large" when $|\text{DFFIT}_i| > 1$ for small to medium-sized data sets and $|\text{DFFIT}_i| > 2\sqrt{p/n}$ for large data sets. We will often just note those DFFIT_i's that are considerable larger than the bulk of the DFFIT_i's.

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- The i^{th} Cook's distance, denoted D_i, is an aggregate measure of the influence of the i^{th} observation on all n fitted values:

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- Look for values of Cook's distance significantly larger than other values; these are cases that have disproportionate influence on the fitted regression surface as a whole.

Review of diagnostics

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  An alternative approach that allows keeping correlated predictors is ridge regression (Chapter 11).
- Deleted residuals $t_i \sim t_{n-p-1}$, so you can formally define an outlier as being larger than $t_{1-\alpha/(2n),n-p-1}$.

Review of diagnostics

- Residual plots. Plots of e_i or t_i vs. $\hat{Y}_i$ and versus each $x_1, \ldots, x_k$ help assess (a) correct functional form, (b) constant variance, and (c) outlying observations. They may also suggest a transformation for a predictor or two.

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  - Heteroscedasticy can be corrected by transforming Y, or else modeling the variance directly (Chapter 11).
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  Added variable plots help figure out functional form of predictors, and whether significance is being driven by one or two points only.

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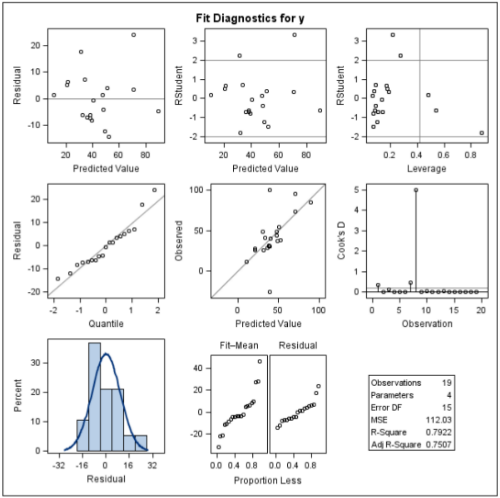
- **Leverages** tell you which points *can potentially* influence the fitted model.
- A **normal Q-Q plot** of the residuals will indicate departures from normality.
- A list of the studentized deleted residuals, leverages, and Cook's distances helps to determine outlying values that may be transcription errors or data anomalies and also indicates those observations that affect the fitted regression surface as a whole.

Standard diagnostic plots

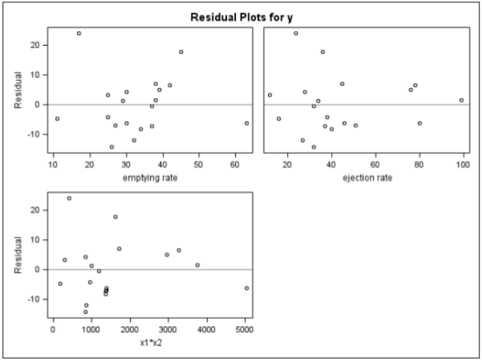
- t_i vs. h_i. Which observations are outlying in **x**-direction, outlying in Y-direction, or both?
- D_i vs. i. Which observations grossly affect fit of regression surface?
- e_i vs. $\hat{Y}_i$ and t_i vs. $\hat{Y}_i$. Constant variance & linearity.
- Y_i vs. $\hat{Y}_i$; how well model predicts its own data. Better models have points close to line $y = x$.
- Normal probability plot of the $e_1, \ldots, e_n$.
- Histogram of $e_1, \ldots, e_n$.
- Plots of e_i vs. each predictor $x_1, \ldots, x_k$.
- One more plot that prof. Hanson never looks at.

An example of diagnostics



Model is $Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_{12} x_{i1} x_{i2} + \epsilon_i$. One highly influential point & one poorly fit.

Residual plots



These look pretty good, except for the one large residual.

Arterial pressure data

```
proc glm;
 model y=x1 x2 x1*x2;
 output out=out cookd=c rstudent=r; run;
proc print; var x1 x2 y c r; run;
-------------------------------------------------------------------
```

Obs	x1	x2	y	c	r
1	45	36	49	0.36904	2.20950
2	30	28	55	0.00383	0.39889
3	11	16	85	0.12052	-0.62921
4	30	46	32	0.00885	-0.60493
5	39	76	26	0.01498	0.51721
6	42	78	28	0.02392	0.66178
7	17	24	95	0.45892	3.31414
8	63	80	26	4.99081	-1.77941
9	25	12	74	0.00724	0.33794
10	32	27	37	0.04100	-1.22324
11	37	37	31	0.01660	-0.71526
12	29	34	49	0.00032	0.12816
13	26	32	38	0.04023	-1.45743
14	38	45	41	0.01271	0.69211
15	38	99	12	0.00817	0.18206
16	25	38	44	0.00422	-0.40213
17	27	51	29	0.02196	-0.70921
18	37	32	40	0.00014	-0.05730
19	34	40	31	0.01371	-0.80210

Obs. 7 has largest arterial pressure. Obs. 8 has relatively small arterial pressure.

Dropping obs. 8 and obs. 7

```
proc glm data=out; model y=x1 x2 x1*x2; run;
--------------------------------------------------------------------
                                    Standard
Parameter         Estimate             Error    t Value    Pr > |t|
Intercept      134.3998664       15.98159869       8.41      <.0001
x1              -2.1330220        0.52215739      -4.09      0.0010
x2              -1.6993299        0.36366865      -4.67      0.0003
x1*x2            0.0333471        0.00928281       3.59      0.0027
--------------------------------------------------------------------
proc glm data=out(where=(c<4)); model y=x1 x2 x1*x2; run;
--------------------------------------------------------------------
                                    Standard
Parameter         Estimate             Error    t Value    Pr > |t|
Intercept      157.5094488       19.79515582       7.96      <.0001
x1              -2.7122125        0.58667658      -4.62      0.0004
x2              -2.7743376        0.69321545      -4.00      0.0013
x1*x2            0.0618590        0.01822201       3.39      0.0044
--------------------------------------------------------------------
proc glm data=out(where=(abs(r)<3)); model y=x1 x2 x1*x2; run;
--------------------------------------------------------------------
                                    Standard
Parameter         Estimate             Error    t Value    Pr > |t|
Intercept      116.3928224       13.52293668       8.61      <.0001
x1              -1.6161083        0.43361763      -3.73      0.0023
x2              -1.4903775        0.28875668      -5.16      0.0001
x1*x2            0.0272510        0.00742428       3.67      0.0025
```

How do 7 and 8 affect the significance and/or magnitude of the effects?