One More Example   Fitting Surface and Curves

Describing Relationships

Idea

Fitting Lines

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Good Fit

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R^2

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MLR

Example: Hardness of Alloy

A group of researchers are studying influences on the hardness of a metal alloy. The researchers varied the percent copper and tempering temperature, measuring the hardness on the Rockwell scale.

The goal is to describe a relationship between our response, Hardness, and our two experimental variables, the percent copper (x_1) and tempering temperature (x_2).

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Example: Hardness of Alloy

Percent Copper	Temperature	Hardness
0.02	1000	78.9
	1100	65.1
	1200	55.2
	1300	56.4
0.10	1000	80.9
	1100	69.7
	1200	57.4
	1300	55.4
0.18	1000	85.3
	1100	71.8
	1200	60.7
	1300	58.9

Example: Hardness of Alloy

Theoretical Relationship:

We start by writing down a theoretical relationship. With one experimental variable, we may start with a line. Extending that idea for two variables, we start with a plane:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

Observed Relationship:

In our data, the true relationship will be shrouded in error.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \text{errors}$$

$$= [\qquad \text{signal} \qquad] + [\text{noise}]$$

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Fitted Relationship:

If we are right about our theoretical relationship, though, and the signal-to-noise ratio is small, we might be able to estimate the relationship:

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2$$

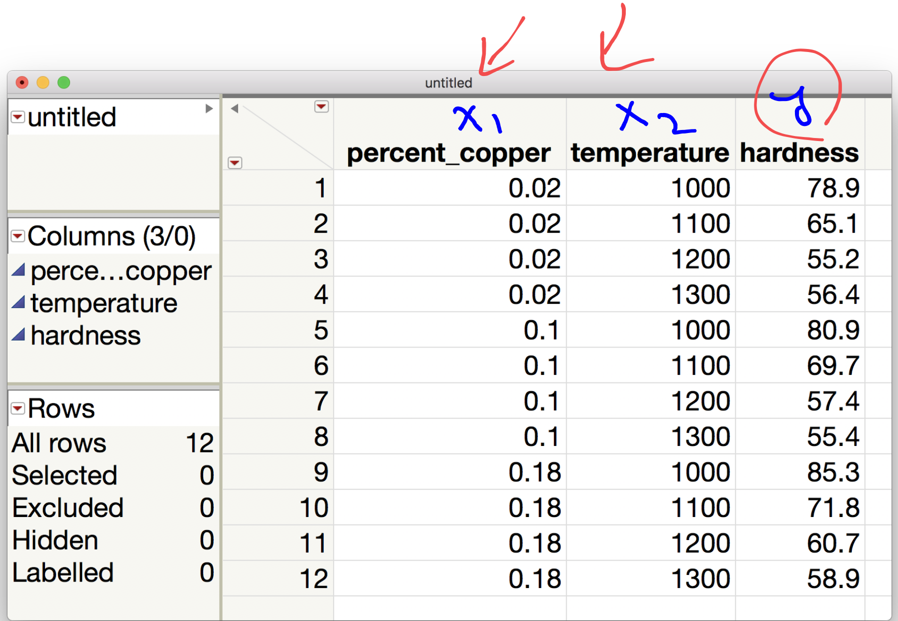
hardness

copper%.

temp.

Example: Hardness of Alloy

Enter the data in JMP



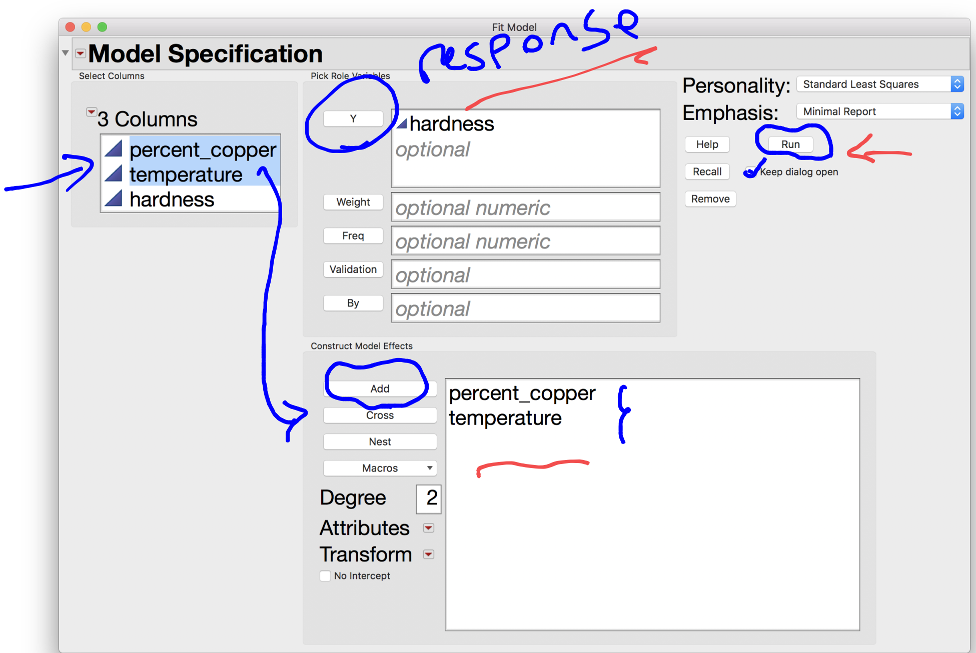
	percent_copper	temperature	hardness
1	0.02	1000	78.9
2	0.02	1100	65.1
3	0.02	1200	55.2
4	0.02	1300	56.4
5	0.1	1000	80.9
6	0.1	1100	69.7
7	0.1	1200	57.4
8	0.1	1300	55.4
9	0.18	1000	85.3
10	0.18	1100	71.8
11	0.18	1200	60.7
12	0.18	1300	58.9

Example: Hardness of Alloy

In JMP, go to

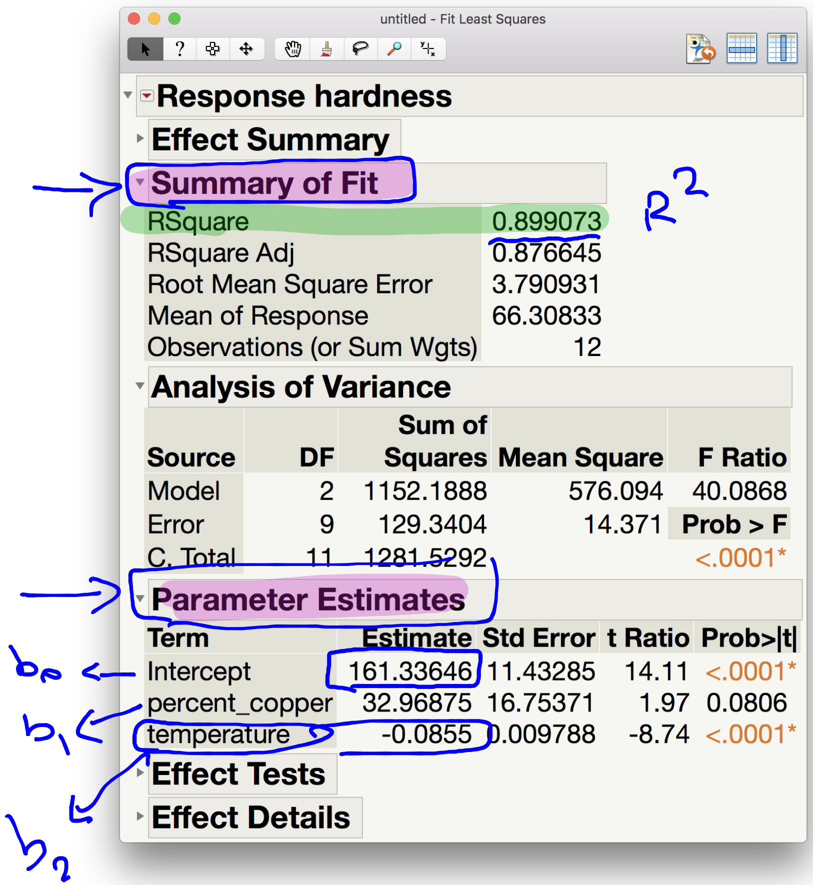
> `Analyze > Fit Model`

to define the model you are fitting:



Example: Hardness of Alloy

After clicking `Run` we get the following model fit results:



Summary of Fit

RSquare	0.899073
RSquare Adj	0.876645
Root Mean Square Error	3.790931
Mean of Response	66.30833
Observations (or Sum Wgts)	12

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	2	1152.1888	576.094	40.0868
Error	9	129.3404	14.371	Prob > F
C. Total	11	1281.5292		<.0001*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	161.33646	11.43285	14.11	<.0001*
percent_copper	32.96875	16.75371	1.97	0.0806
temperature	-0.0855	0.009788	-8.74	<.0001*

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Example: Hardness of Alloy

From this output, we can get the value of R^2, the coeffecient of determination:

Summary of Fit

RSquare	0.899073
RSquare Adj	0.876645
Root Mean Square Error	3.790931
Mean of Response	66.30833
Observations (or Sum Wgts)	12

Since $R^2 = 0.899073$, we can say

> 89.9074% of the variability in the hardness we observed can be explained by its relationship with temperature and percent copper.

Example: Hardness of Alloy

From this output, we can get the sum of squares.

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	2	1152.1888	576.094	40.0868
Error	9	129.3404	14.371	**Prob > F**
C. Total	11	1281.5292		<.0001*

This "Analysis of Variance" table has the same format across almost all textbooks, journals, software, etc. In our notation,

- $SSR = 1152.1888$
- $SSE = 129.3404$
- $SSTO = 1281.5292$

We can use these for lots of purposes. In this class, we have seen that we can get R^2:

$$R^2 = 1 - \frac{SSE}{SSTO} = 1 - \frac{129.3404}{1281.5292} = 0.8990734$$

Example: Hardness of Alloy

The parameter estimates give us the fitted values used in our model:

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	161.33646	11.43285	14.11	<.0001*
percent_copper	32.96875	16.75371	1.97	0.0806
temperature	-0.0855	0.009788	-8.74	<.0001*

$b_0 =$ $b_1 =$ $b_2 =$

Since we defined percent copper as x_1 earlier and temperature as x_2 then we can write:

$$\hat{y} = 161.33646 + 32.96875 \cdot x_1 - 0.0855 \cdot x_2$$

We can use this to get fitted values. If we use temperature of 1000 degrees and percent copper of 0.10 then we would predict a hardness of

$$\hat{y} = 161.33646 + 32.96875 \cdot (0.10) - 0.0855 \cdot (1000)$$

$$= 161.33646 + 3.296875 - 85.5$$

$$= 79.13333$$

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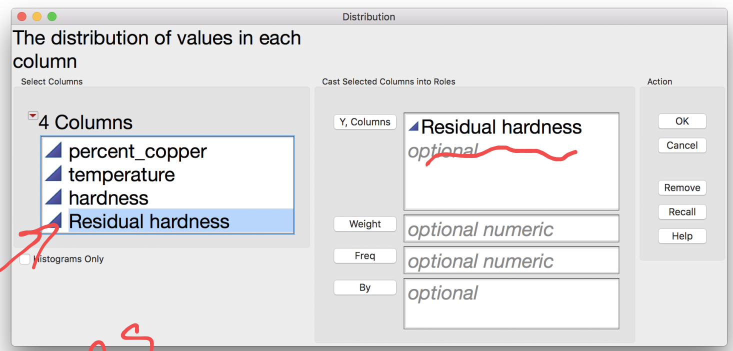
Example: Hardness of Alloy

While our model looks pretty good, we still need to check a few things involving residuals. We can save our residuals from the model fit drop down and analyze them.

From Analyze > Distribution:



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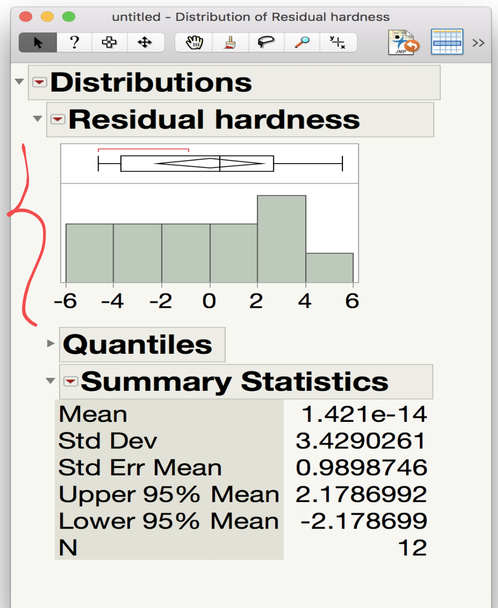
Example: Hardness of Alloy

There aren't many residuals here (just 12) but we would like to make sure that the histogram has rough bell-shape (normal residuals are good). I would call this one inconclusive.



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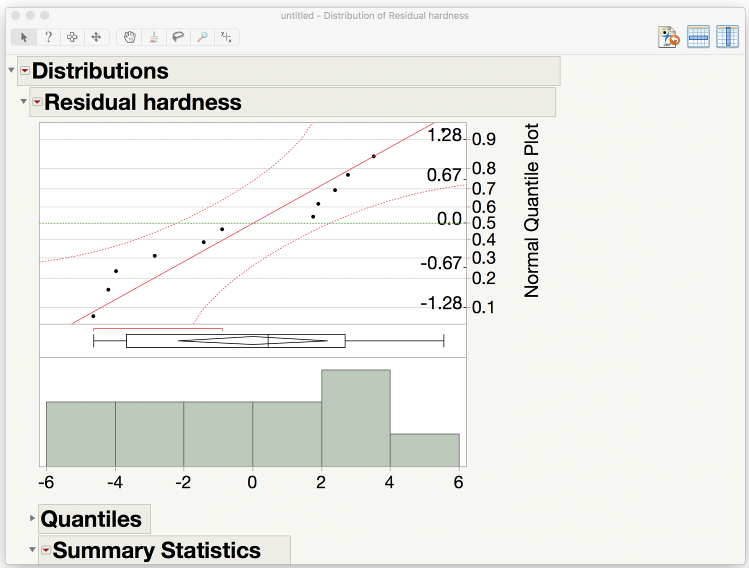
Example: Hardness of Alloy

Another way to check if the residuals are approximately normal is to compare the quantiles of our residuals to the theoretical quantiles of the true normal distribution.

From the dropdown menu, choose Normal Quantile Plot to get:



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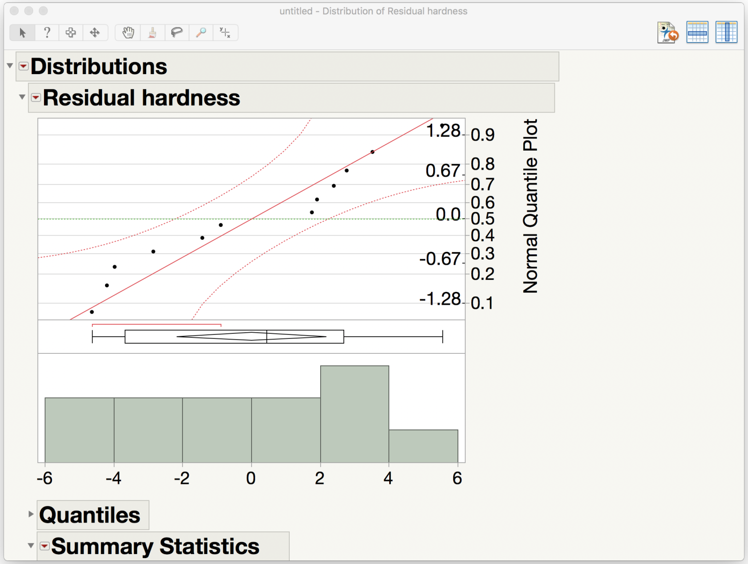
Example: Hardness of Alloy



- If the points all fall on the line, then the residuals have the same spread as the normal distribution (i.e., the residuals follow a bell-shape, which is what we want).
- If they stay within the curves, then we can say the residuals follow a rough bell shape (which is good).
- If points fall outside the curves, our model has problems (which is bad).

Transformations

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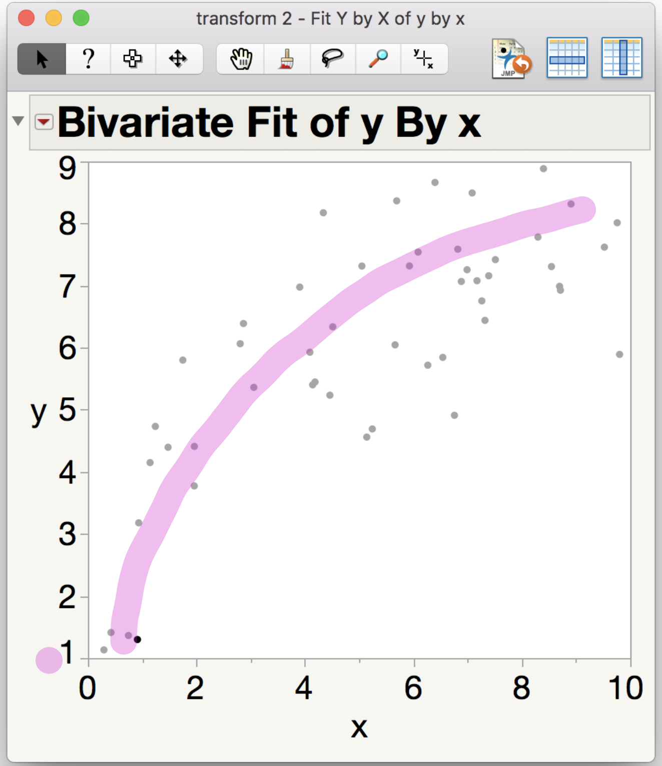
Transformations: Fitting complicated relationships

Consider the simulated dataset 'transform.csv' in the lecture module. Here's the scatterplot:



Transformations: Fitting complicated relationships

Consider the residual plot you would get by trying to fit a line. What would that look like?

Now consider the residual plot you would get by trying to fit a quadratic. What would that look like?

What can we do about the size of the residuals??

We need a function that can both adjust the scale our responses and account for the curve!!

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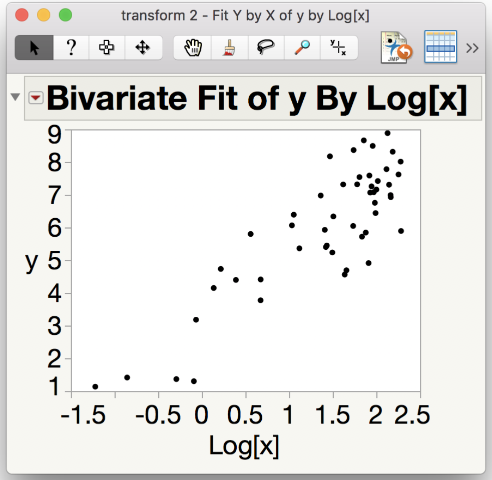
Transformations: Fitting complicated relationships

One possible function that could do that: $ln(x)$.



Transforming our variables can allow us to get better fits, but you need to be careful about the meaning of the relationship. For instance, the slope now means "the change in the response when *the natural log of x is increased by 1* - the relationship to x itself is not always easy to translate back.

Dangers in Fits

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Dangers in Fits

Overfitting

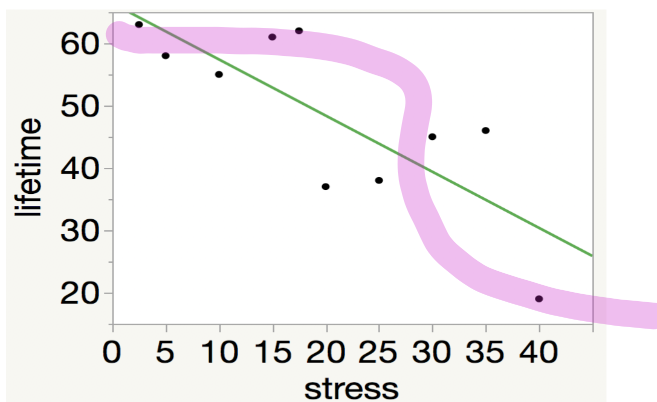
Dangers in Fitting Relationships

Example: Stress and Lifetime of Bars

Consider the bars example again

stress (kg/mm^2)	2.5	5.0	10.0	15.0	17.5	20.0	25.0	30.0	35.0	40.0
lifetime (hours)	63	58	55	61	62	37	38	45	46	19

Here's the linear fit:



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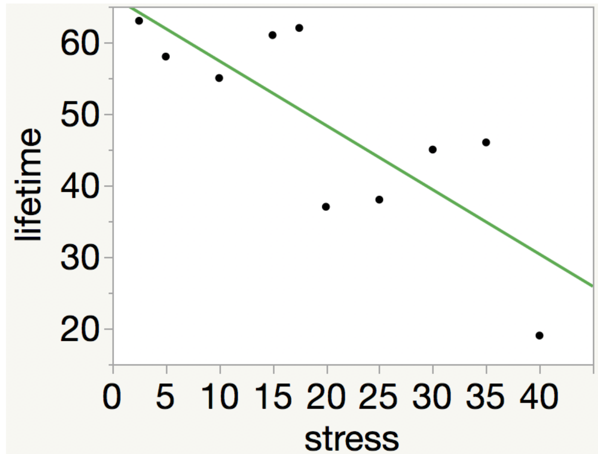
Overfitting

Dangers in Fitting Relationships

Example: Stress and Lifetime of Bars



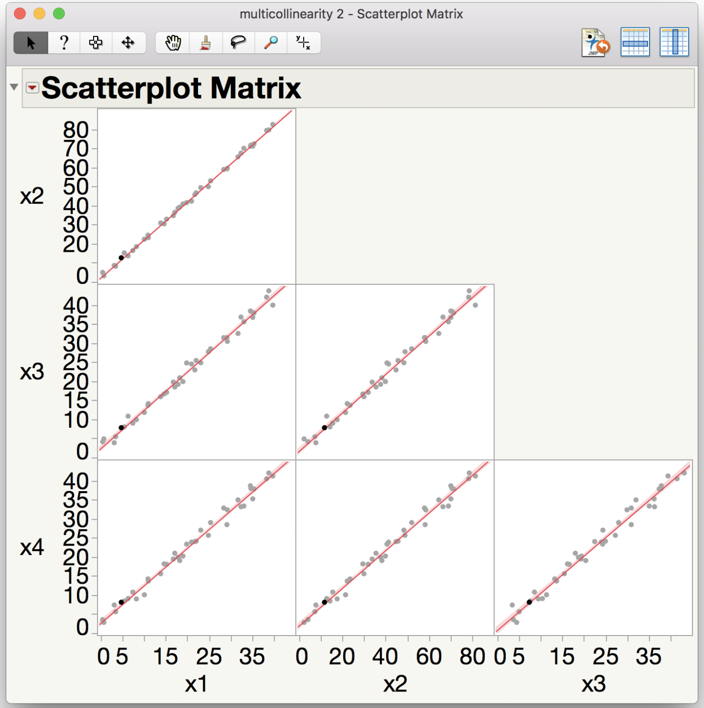
The fitted line doesn't touch all the points, but we can push our relationship further by adding $(stress)^2$, $(stress)^3$, $(stress)^4$, and so on.

Everytime we add a new term to the polynomial, we give the fitted relationship the ability to make one more turn.

This leads to a problem called **overfitting**: our model is just following *the data*, including the errors, instead of uncovering *the true relationship*.

Multicollinearity

Multicollinearity occurs when you have strongly correlated experimental variables.



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Multicollinearity

Multicollinearity can lead to several problems:

- Since the variables are all related to each other, the impact each variable has in the relationship to the response becomes difficult to determine
- Since the disentangling the relationships is difficult, the estimates of the slopes for each variable become very sensitive (different samples lead to very different estimates)
- Since the correlated experimental variables will have similar relationships to the response, most of them are not needed. Including them leads to an overfit.

Ultimately while it may look like a good fit on paper, the model will be inaccurate.

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Finding the Best Fit

- Again, we can use the **Least Squares** principle to find the best estimates, b_0, b_1, and b_2.
- The calculations are fairly advanced now that we have three values to estimate,
- so these calculations are usually done in statistical software (like JMP).

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Wrapup

Judging The Fit

- Not all Theoretical Relationships we may imagine are real!
- Perhaps a better relationship could be found using

$$y = \beta_0 + \beta_1 x_1 + \beta_2 \ln(x_2)$$

- We determine which relationships to try by examining plots of the data, fit statistics (like R^2), and plots of residuals.
- Be careful of overfitting and multicollinearity (when the experimental variables are correlated).