

# Multiple Regression: A Model for the Mean

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STRUCTURAL VS. DATA-BASED MULTICOLLINEARITY

WEIGHTED REGRESSION

NONLINEAR REGRESSION

# Types of Multicollinearity

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## **Data-Based**

The inclusion of two or more explanatory variables that are highly correlated

This could be from

- a mistake in the experimental design  
(e.g.  $x_1$  is whether subject has down syndrome,  $x_2$  is # of chromosome 21s)
- an experiment (or observational study) in which the data cannot be manipulated to lower the correlation  
(can you come up with an example?)

## **Structural-Based**

Comes from the inclusion of interaction terms or from other transformations (such as polynomial terms)

# Data-Based Multicollinearity

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# Data-Based Multicollinearity

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The inclusion of additional explanatory variables has several effects

**We've talked about some of the benefits:**

- Possibly improving model fit
- Decreasing the (estimated) variance  $s^2$
- Controlling for confounders (in an observational study)

**However, there are some definite costs:**

- $\widehat{var}(\hat{\beta}_j)$  tends to increase as more terms are added
- Coefficient estimates depend on what terms are in the model

“variance considerations”

“design considerations”

The “benefits” vs. “costs” depends on the specifics of the explanatory variables

# Variance Considerations

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# Variance Considerations

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When interested in inference about a particular parameter, we would form:

$$\hat{\beta}_j \pm t_{\alpha/2, n-(p+1)} \sqrt{\widehat{var}(\hat{\beta}_j)}$$

After some computations, we can show that

$$\widehat{var}(\hat{\beta}_j) = \frac{s^2}{(n-1)\widehat{var}(x_j)} \cdot \frac{1}{1-R_j^2}$$

$R_j^2$  is the “coefficient of determination” of a multiple regression with  $x_j$  as the response and the other  $x_k, k \neq j$  as the explanatory variables

(In other words,  $R_j^2$  is the proportion of variance in  $x_j$  that is explained by a linear model with all other explanatory variables)

Let’s discuss each of these terms in isolation

The relative sizes of each term determines the “benefit” vs. “cost”

# Variance Considerations

$$\widehat{var}(\hat{\beta}_j) = \frac{s^2}{(n-1)\widehat{var}(x_j)} \cdot \frac{1}{1-R_j^2}$$

Reminder: The variance  $\sigma^2$  is estimated by  $s^2 = \text{MSE}$ , which can be found on the ANOVA table

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	4	3.988723E13	9.9718076E12	88.94	<.0001
Error	24	2.6908501E12	112118754091		
Corrected Total	28	4.257808E13			

Where  $\text{MSE} = \frac{1}{n-(p+1)} \sum_{i=1}^n (Y_i - \hat{\mu}\{Y_i|X_i\})^2$

As we add more terms to the model

- $\sum_{i=1}^n (Y_i - \hat{\mu}\{Y_i|X_i\})^2$  goes down

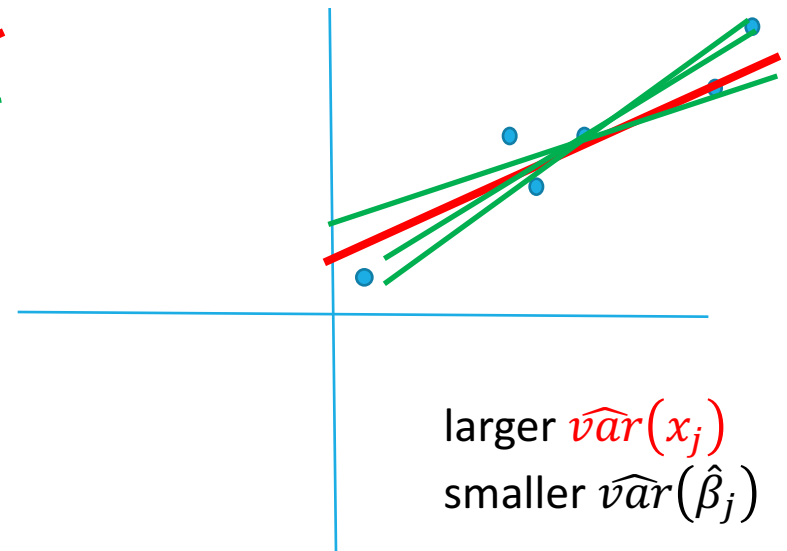
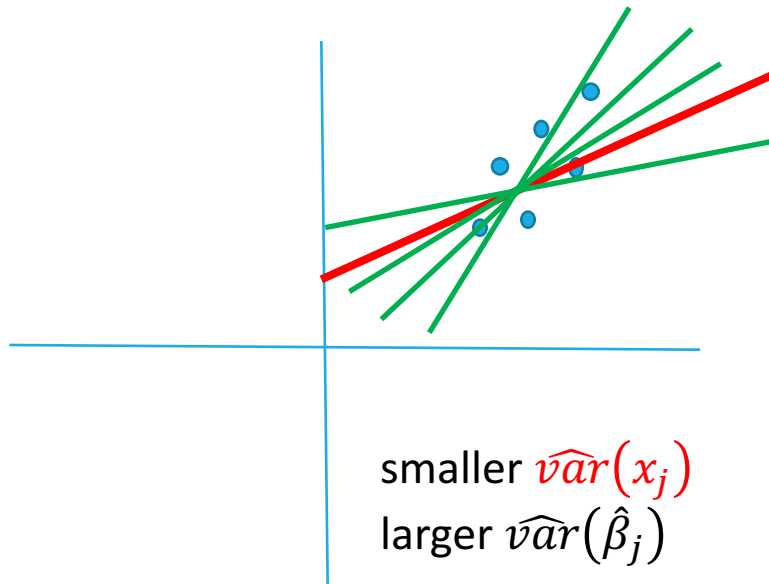
- $\frac{1}{n-(p+1)}$  goes up

**Net result on  $s^2$ :** Depends on the relative size (e.g. F-test)

# Variance Considerations

$$\widehat{\text{var}}(\hat{\beta}_j) = \frac{s^2}{(n-1)\widehat{\text{var}}(x_j)} \cdot \frac{1}{1-R_j^2}$$

The variability of the explanatory variable contributes to the variance





# Variance Considerations

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$$\widehat{var}(\hat{\beta}_j) = \frac{s^2}{(\textcolor{red}{n}-1)\widehat{var}(x_j)} \cdot \frac{1}{1-R_j^2}$$

The term  $\frac{1}{\textcolor{red}{n}-1}$  goes down as  $\textcolor{red}{n}$  increases (a general consistency property)

# Variance Considerations

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$$\widehat{var}(\hat{\beta}_j) = \frac{s^2}{(n-1)\widehat{var}(x_j)} \cdot \frac{1}{1-R_j^2} = \frac{s^2}{(n-1)\widehat{var}(x_j)} \cdot VIF_j$$

$$VIF_j = \frac{1}{1-R_j^2}$$

Here:

$R_j^2$  increases  $\rightarrow VIF_j$  increases  $\rightarrow \widehat{var}(\hat{\beta}_j)$  increases

As this relationship is so direct, it goes by a special term:

**VARIANCE INFLATION FACTOR (VIF)**

# Design Considerations

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# Data-Based Multicollinearity

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The inclusion of additional explanatory variables has several effects

**We've talked about some of the benefits:**

- Possibly improving model fit
- Decreasing the (estimated) variance  $s^2$
- Controlling for confounders (in an observational study)

**However, there are some definite costs:**

- $\widehat{var}(\hat{\beta}_j)$  tends to increase as more terms are added
- Coefficient estimates depend on what terms are in the model

“design considerations”



The “benefits” vs. “costs” depends on the specifics of the explanatory variables

# Design Considerations: Controlling for confounders

```
PROC GLM DATA = population PLOTS = ALL;  
  MODEL crime = police / SOLUTION;  
RUN;
```

Parameter	Estimate	Standard Error	t Value	Pr >  t
Intercept	121.8850878	63.91254453	1.91	0.0726
police	0.2735152	0.10408009	2.63	0.0171

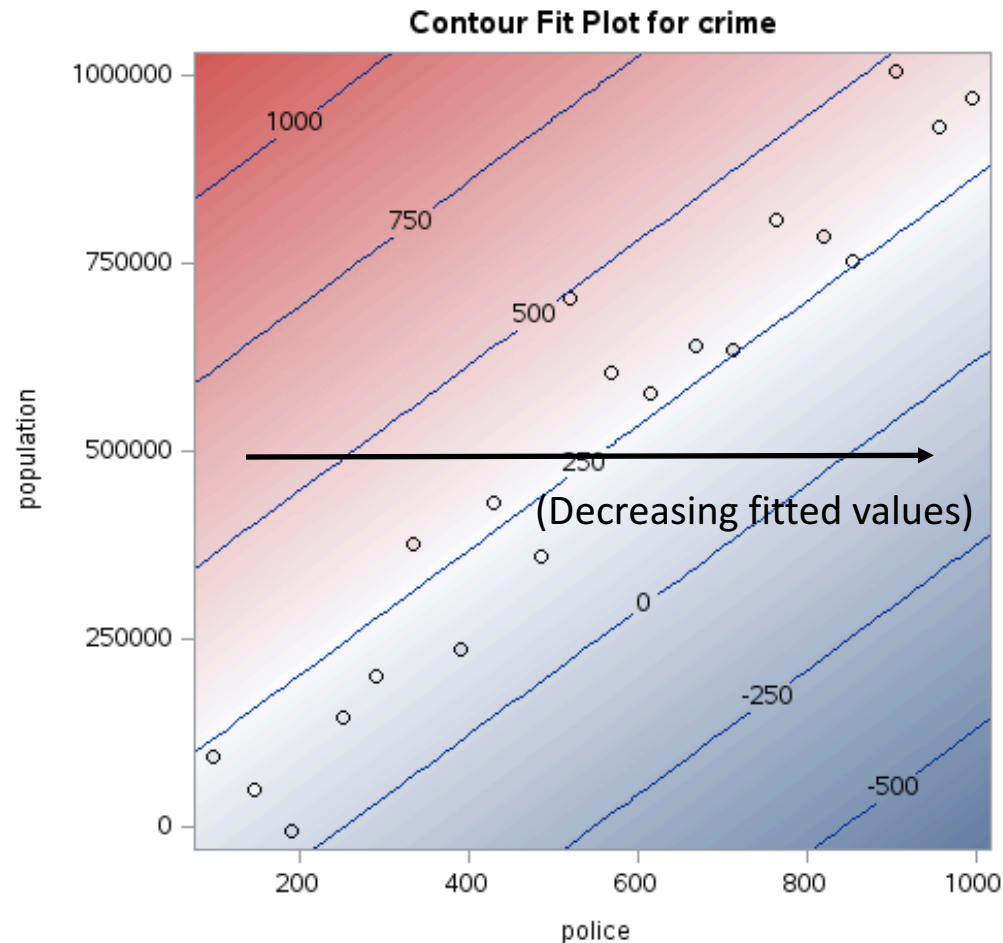
```
PROC GLM DATA = population PLOTS = ALL;  
  MODEL crime = police population / SOLUTION;  
RUN;
```

(From  
9c\_linearRegressionDarren)

Parameter	Estimate	Standard Error	t Value	Pr >  t
Intercept	213.5840719	52.54467999	4.06	0.0008
police	-0.8427494	0.29009519	-2.91	0.0099
population	0.0010162	0.00025463	3.99	0.0009

# Design Considerations: Controlling for confounders

This is a “contour”  
plot.  
Note: “Crime” is  
not plotted here



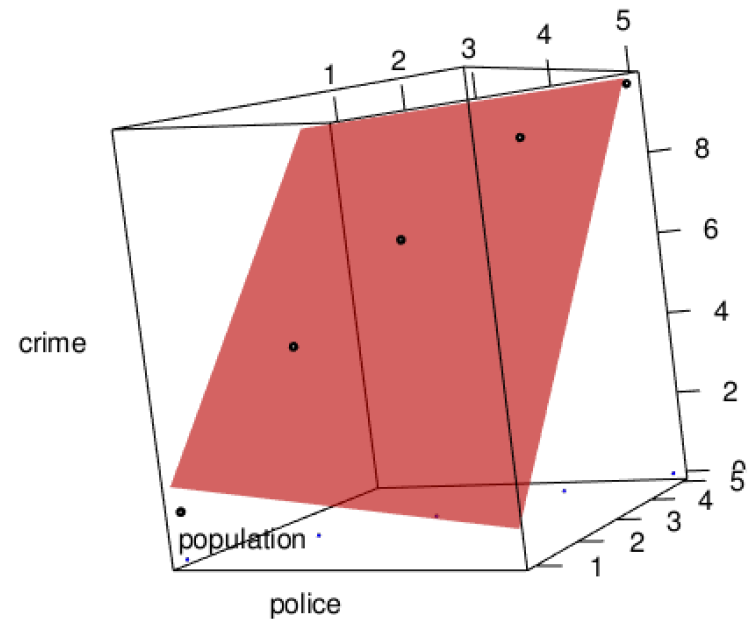
(From  
9c\_linearRegressionDarren)

# Go to Visualization...

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In-class experiment with code:

**12a\_regressionInvestigation.R**



# Design Considerations: Experimental Design

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A big initiative in classical experimental design was to create designs that are **ORTHOGONAL**

With an orthogonal design, each of the explanatory variables are uncorrelated

This has (had) some benefits

- (estimation is computationally easier and more stable)
- The coefficient estimates for an explanatory variable is the same whether or not other explanatory variables are included
- The sums of squares are maximally reduced



# Example of Orthogonal Design

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Suppose we have a continuous response

A “fully balanced” design will be orthogonal

An important example of this is a **FACTORIAL DESIGN** with equal number of observations at each experiment condition

**Example:** Suppose we have 3 categorical explanatory variables  $x_1, x_2, x_3$  each taking two levels

Assign the levels of the explanatory variables to -1 or 1

The “factorial design” is looking at all combinations of the explanatory variables

Then, the design matrix for all interactions  $\mathbb{X}$  is **ORTHOGONAL** in the sense of matrices, that is  $\mathbb{X}^T \mathbb{X} = n \cdot I$ , where  $I$  is the identity matrix

# Design Considerations: Observational Studies

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Suppose we have two explanatory variables  $x_1$  and  $x_2$

If  $x_1$  and  $x_2$  are not orthogonal, then the estimate of  $\beta_1$  will be affected by whether or not  $x_2$  is included (and vice-versa)

If  $x_1$  and  $x_2$  both are highly positively correlated, then they really are measuring some latent factor, call it  $z$ , where  $z \approx x_1$  and  $z \approx x_2$

If the true state of nature for the response is

$$\mu\{Y|Z\} = \beta_0 + \beta z$$

Then if we estimate the model:

$$\mu\{Y|X\} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \approx \beta_0 + (\beta_1 + \beta_2) z$$

So, by including both  $x_1$  and  $x_2$ , we are effectively estimating  $(\beta_1 + \beta_2) \approx \beta$

This issue is that many different  $\beta_1, \beta_2$  will satisfy this

# Design Considerations: Observational Studies

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When using least squares to estimate the coefficients in the model

$$\mu\{Y|X\} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

the particular coefficients tend to exhibit a “heroic cancellation”

(The interpretation of a coefficient is “given the other terms in the model”)

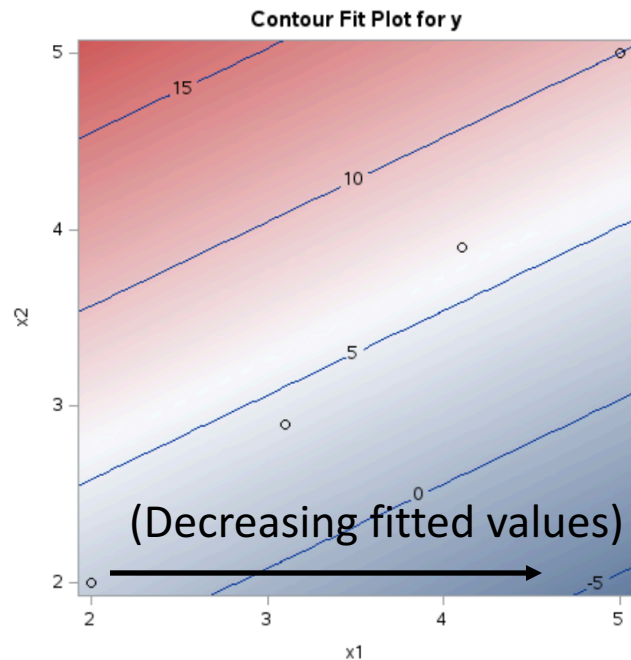
Example:  $\hat{\beta}_1$  will be a large positive number,  $\hat{\beta}_2$  will be a large negative number

This behavior is attributable to the fitted surface “paying more attention” to the  $Y$  direction than the  $x_1, x_2$  direction

Let’s look at a very simple example..

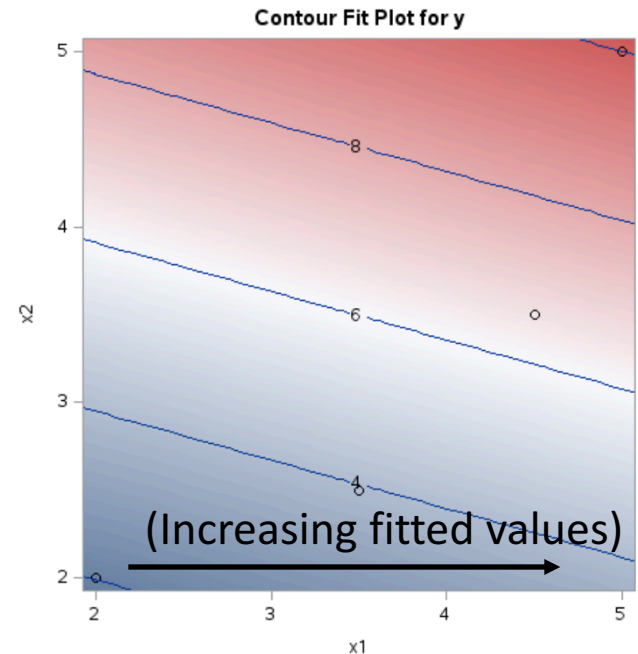
```
DATA multi;
  INPUT x1 x2 y;
  DATALINES;
    2    2    2
    3.5  2.5  4
    4.5  3.5  6.5
    5    5    10
  ;
```

Parameter	Estimate	Standard Error	t Value	Pr >  t
Intercept	-3.275000000	0.19202864	-17.05	0.0373
x1	-2.425000000	0.55957573	-4.33	0.1444
x2	5.075000000	0.55957573	9.07	0.0699



```
DATA multi;
  INPUT x1 x2 y;
  DATALINES;
    2    2    2
    3.1  2.9  4
    4.1  3.9  6.5
    5    5    10
  ;
```

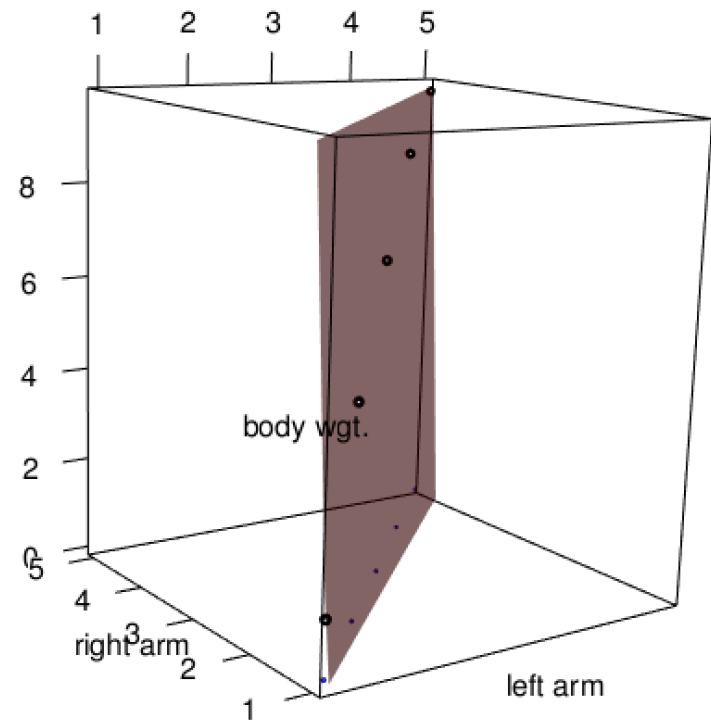
Parameter	Estimate	Standard Error	t Value	Pr >  t
Intercept	-3.275000000	0.19202864	-17.05	0.0373
x1	0.575000000	0.11456439	5.02	0.1252
x2	2.075000000	0.11456439	18.11	0.0351



# Go to Visualization...

In-class experiment with code:

[12a\\_regressionInvestigation.R](#)



# Multicollinearity & Predictions

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# Back to Decomposing the Prediction Accuracy

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- The true relationship between  $Y$  and  $X$  is:

$$Y = \mu\{Y|X\} + \varepsilon$$

We want to predict a new  $Y$  with our linear model  $(\widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j x_j)$

Smaller values of  $Y - (\widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j x_j)$  indicate we did a better job. This can be decomposed as:

$Y - (\widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j x_j) = \text{Approximation error} + \text{Estimation error} + \text{Irreducible Error}$ , where:

- Approximation error:  $\mu\{Y|X\} - (\beta_0 + \sum_{j=1}^p \beta_j x_j)$
- Estimation error:  $(\beta_0 + \sum_{j=1}^p \beta_j x_j) - (\widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j x_j)$
- Irreducible error:  $\varepsilon$

# Multicollinearity and Predictions

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Multicollinearity is somewhat less a concern when the primary goal is prediction

$$Y - \left( \widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j x_j \right) = \text{Approximation error} + \text{Estimation error} + \text{Irreducible Error},$$

- Approximation error:  $\mu\{Y|X\} - \left( \beta_0 + \sum_{j=1}^p \beta_j x_j \right)$
- Estimation error:  $(\beta_0 + \sum_{j=1}^p \beta_j x_j) - (\widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j x_j)$   
[Estimation error of  $\hat{\mu}$ :  $(\mathbb{E}\hat{\mu}\{Y_i|X_i\} - \mu\{Y_i|X_i\})^2 + \mathbb{E}(\hat{\mu}\{Y_i|X_i\} - \mathbb{E}\hat{\mu}\{Y_i|X_i\})^2$  ]
- Irreducible error:  $\varepsilon$
- As  $p$  increases, approximation error tends to decrease
- As  $p$  increases, estimation error tends to increase

( $\hat{\beta}_j$  is unbiased and  $\widehat{var}(\hat{\beta}_j)$  increases with more terms based on previous discussion)



# Example: Kleiber's Law

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# Example: Kleiber's Law

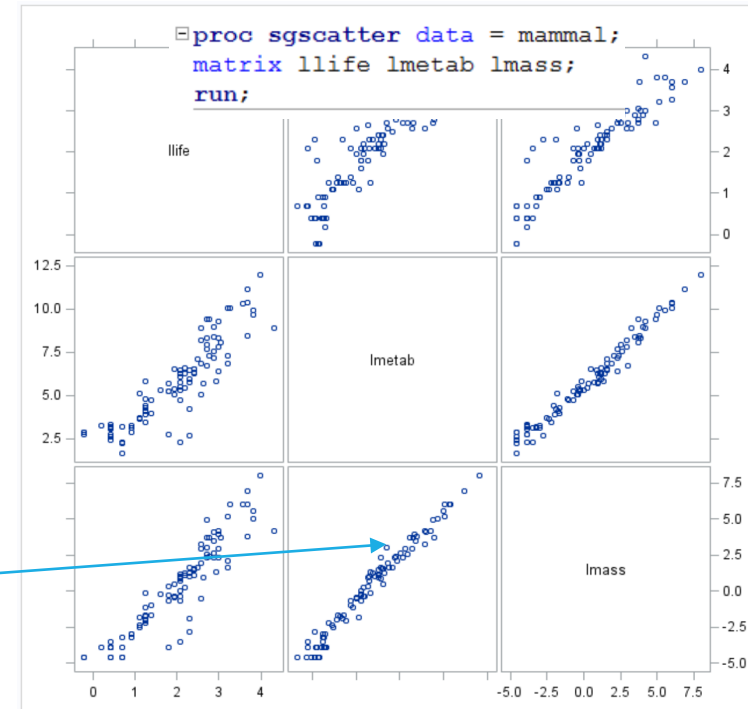
```
DATA mammal;
  INPUT CommonName $ Species $ Mass Metab Life;
  DATALINES;
  Echidna Tachiglossus_aculeatus 2.500 302.00 14
  Long-beaked_echidna Zaglossus_bruijnii 10.300 594.00 20
  Platypus Ornithorhynchus_anatinus 1.300 229.00 9
  Opossum Lutreolina_crassicaudata 0.812 196.00 5
  South_American_opossum Didelphis_marsupialis 1.330 299.00 6
  Virginia_opossum Didelphis_virginiana 3.260 519.00 8
  Australian_marsupial Antechinus_macdonnellensis 0.014 9.00 2
  Marsupial Antechinus_stuartii 0.004 17.60 2.5
  Marsupial Antechinus_laniger 0.009 5.17 2
  Marsupial_rat Dasyuroides_byrnei 0.089 37.40 3
  Bandicoot Isodon_macroonurus 1.000 201.00 8
  Long-nosed_bandicoot Perameles_nasuta 0.645 153.00 7
  Fat-tailed_dunnart Sminthopsis_crassicaudata 0.015 9.64 2
  Australian_marsupial Planigale_maculata 0.013 13.70 1.5
  Tasmanian_devil Sacrophilus_harrisii 5.050 628.00 10
  Brushtail_possum Trichosurus_vulpecula 1.980 306.00 8
  Kangaroo Macropus_robustus 4.690 694.00 11
  Red_kangaroo Macropus_rufus 40.000 4000.00 15
  Tammar_wallaby Macropus_eugenii 4.800 671.00 11
  Sloth Bradypus_variegatus 3.790 331.00 19
  Armadillo Dasypus_novemcinctus 3.320 384.00 10
  Pangolin Manis_tricuspis 2.730 440.00 8
```

```
data mammal;
  set mammal;
  llife = log(life);
  lmetab = log(metab);
  lmass = log(mass);
;
```

**Kleiber's Law:**  
 $\text{metabolism} \propto \text{mass}^{3/4}$

```
proc reg data = mammal;
  model llife = lmass lmetab / vif;
run;
```

(Note: Using **PROC CORR** you can create the correlation matrix among all the explanatory variables)



Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr >  t
Intercept	1	4.25340	0.52284	8.14	<.0001
lmass	1	0.61670	0.07161	8.61	<.0001
lmetab	1	-0.41438	0.09312	-4.45	<.0001

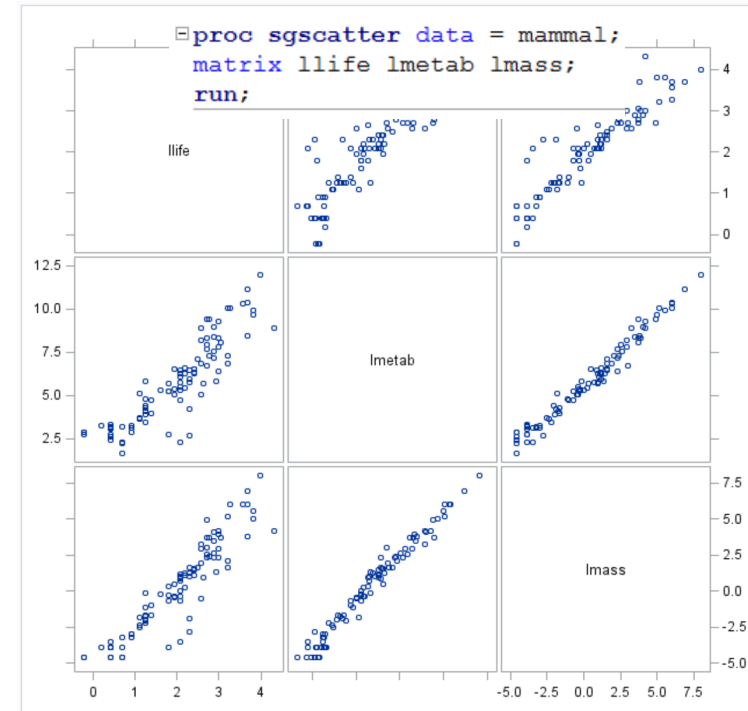
34.88426  
 34.88426

# Confidence Intervals for Coefficients

```
DATA mammal;
  INPUT CommonName $ Species $ Mass Metab Life;
  DATALINES;
Echidna Tachiglossus_aculeatus 2.500 302.00 14
Long-beaked_echidna Zaglossus_bruijnii 10.300 594.00 20
Platypus Ornithorhynchus_anatinus 1.300 229.00 9
Opossum Lutreolina_crassicaudata 0.812 196.00 5
South_American_opossum Didelphis_marsupialis 1.330 299.00 6
Virginia_opossum Didelphis_virginiana 3.260 519.00 8
Australian_marsupial Antechinus_macdonnellensis 0.014 9.00 2
Marsupial Antechinomus_stuartii 0.004 17.60 2.5
Marsupial Antechinomus_laniger 0.009 5.17 2
Marsupial_rat Dasyuroides_byrnei 0.089 37.40 3
Bandicoot Isodon_macroonurus 1.000 201.00 8
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Sloth Bradypus_variegatus 3.790 331.00 19
Armadillo Dasypus_novemcinctus 3.320 384.00 10
Pangolin Manis tricuspis 2.730 440.00 8
;

data mammal;
  set mammal;
  llife = log(life);
  lmetab = log(metab);
  lmass = log(mass);
;

proc reg data = mammal;
  model llife = lmass lmetab / vif clb;
run;
```



Parameter Estimates							
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr >  t	Variance Inflation	95% Confidence Limits
Intercept	1	4.25340	0.52284	8.14	<.0001	0	3.21468 5.29212
lmass	1	0.61670	0.07164	8.61	<.0001	34.88426	0.47444 0.75896
lmetab	1	-0.41438	0.09312	-4.45	<.0001	34.88426	-0.59939 -0.22938

Confidence Interval:  $\hat{\beta}_j \pm t_{\alpha/2, n-p} \sqrt{\widehat{var}(\hat{\beta}_j)}$

# Possible Remediation

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It is provably impossible in an observational study to use only the data to decide whether you should use mass or metabolism

The inclusion of both will lead to a nonsensical inference

What is really happening is that both mass and metabolism seem to be different aspects of the same underlying quantity (total # of cells)

As this quantity wasn't directly measured, it is called it a LATENT FACTOR

We can do one of the following:

- Use subject matter expertise to choose which explanatory variable to use
- Use something like principal components to estimate the latent factor (or even more simply use a particular linear combination)
- Use 'ridge' regression to constrain estimates to prevent heroic cancellation

# Structural-Based Multicollinearity

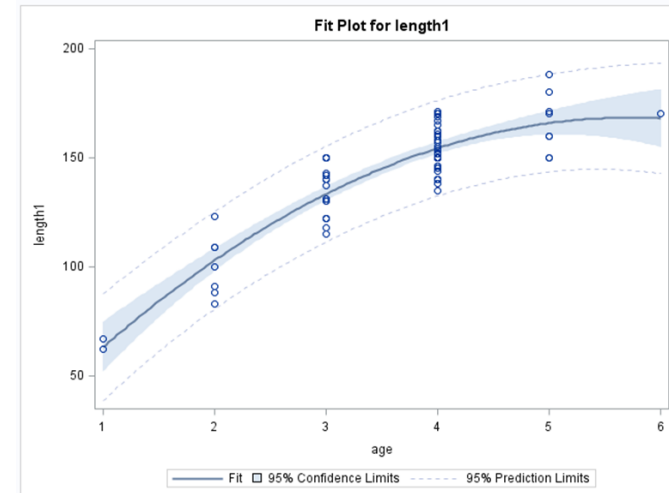
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# Structural-Based Multicollinearity

Let's examine the relationship between a tuna's age and tail length

$$\mu\{Y_i|age_i\} = \beta_0 + \beta_1 age_i + \beta_2 age_i^2$$

We will consider a quadratic polynomial after a visualizing the data set



Parameter Estimates						
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr >  t	Variance Inflation
Intercept	1	13.62238	11.01638	1.24	0.2201	0
age	1	54.04931	6.48884	8.33	<.0001	23.44081
age2	1	-4.71866	0.94396	-5.00	<.0001	23.44081

# Structural-Based Multicollinearity

As large VIFs increase the standard errors, it would be beneficial to decrease them

One solution is via **STANDARDIZATION**

Variable	N	Mean	Std Dev	Minimum	Maximum
age	78	3.6282051	0.9273475	1.0000000	6.0000000
length1	78	143.6025641	24.1366993	62.0000000	188.0000000
age2	78	14.0128205	6.3746527	1.0000000	36.0000000

```
proc means data = bluefinn2;
run;

data bluefinn3;
set bluefinn2;
s_age = (age - 3.628) / .9273;
s_age2 = s_age**2;
;

proc reg data = bluefinn3;
model length1 = s_age s_age2 / vif clb;
run;
```

Parameter Estimates						
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr >  t	Variance Inflation
Intercept	1	13.62238	11.01638	1.24	0.2201	0
age	1	54.04931	6.48884	8.33	<.0001	23.44081
age2	1	-4.71866	0.94396	-5.00	<.0001	23.44081

Before standardization

Parameter Estimates								
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr >  t	Variance Inflation	95% Confidence Limits	
Intercept	1	147.60440	1.47216	100.26	<.0001	0	144.67170	150.53710
s_age	1	18.37044	1.32661	13.85	<.0001	1.13943	15.72769	21.01319
s_age2	1	-4.05751	0.81170	-5.00	<.0001	1.13943	-5.67449	-2.44053

After standardization

## Downside:

Interpretation is now in “standard deviations away from the mean of age” instead of years

# Conclusion

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Multicollinearity is a term that describes the linear correlation between explanatory variables.

Multicollinearity can have the effect of inflating the variance of the estimate. This has the effect of having less confidence in the value of the estimate through wider confidence intervals. It will also inflate the p-values and make your tests less powerful.

The variance inflation factor (VIF) is a common measure of multicollinearity. A typical tolerance is equal to  $1/\text{VIF}$ .

There are two types of collinearity: data based and structural.

Methods of dealing with multicollinearity include deleting redundant variables and/or designing a better experiment. If the multicollinearity is structural then centering / standardizing the variables may help.



# Weighted Regression

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# Multiple Regression: Constant Variance

The regression of  $Y$  on  $X_1$  and  $X_2$  is  $\mu\{Y|X_1, X_2\}$ .

**Regression plane:**  $\mu\{\text{flowers}|\text{light}, \text{time}\} = \beta_0 + \beta_1 \text{light} + \beta_2 \text{time}$

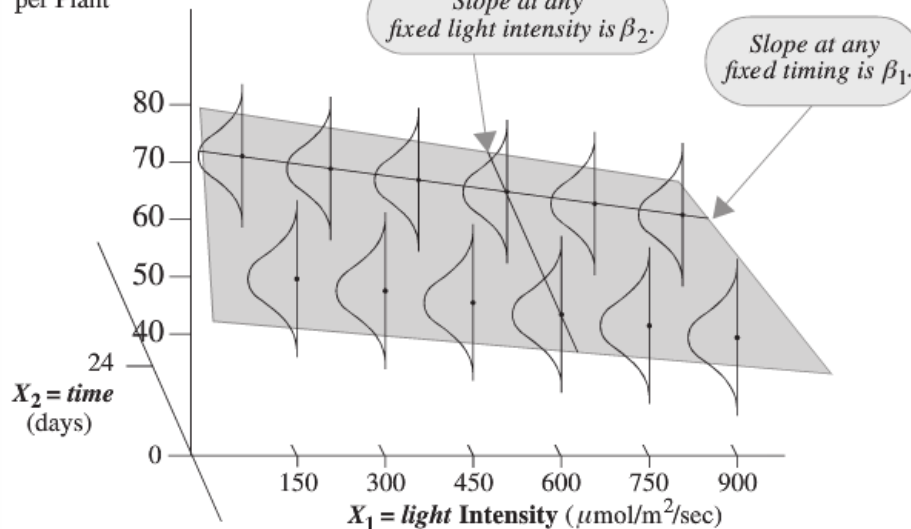
$\text{Var}\{\text{flowers} | \text{light}, \text{time}\} = \sigma^2$

## DISPLAY 9.5

Model for the regression surface of flowers per plant under 12 treatment levels as a regression plane

**Regression plane:**  $\mu\{\text{flowers}|\text{light}, \text{time}\} = \beta_0 + \beta_1 \text{light} + \beta_2 \text{time}$

$Y = \text{flowers}$   
per Plant



“Constant Variance Assumption”  
(homoscedasticity)

This assumption is needed for the inferential tools developed in the next Chapter (intervals, tests, etc.)

# Weighted Regression

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The alternative scenario is sometimes called heteroscedasticity

Multiple regression takes an average of all the observations

If the observations have unequal variances, we should include down weight the more variable observations in this average

Looking at the least squares problem:

$$\text{minimize } \sum_{i=1}^n (Y_i - (\beta_0 + \sum_{j=1}^p X_{ij}\beta_j))^2$$

This implicitly equally weights each observation

Suppose the variance of the  $i^{th}$  observation is  $\sigma_i^2$ . Then weighting makes sense

$$\text{minimize } \sum_{i=1}^n w_i (Y_i - (\beta_0 + \sum_{j=1}^p X_{ij}\beta_j))^2$$

And with weights  $w_i = 1/\sigma_i^2$

# Weighted Regression

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Some typical scenarios when weighted regression is appropriate

- The response is estimated and some reasonable standard errors are available

**Example:** In particle physics, highly sensitive detectors are used to make measurements. These detectors tend to come with estimates of the variability in the measurements

- Responses themselves are averages and we know the total number of terms

**Example:** For privacy reasons, we can only get the total number of drug users in a school instead of whether particular students use drug

- It is sensible that both 1) the variance is proportional to  $X$  and 2) the  $X, Y$  relationship is linear

**Example:** A person is counting grouse in a field ( $Y$ ) and the time of day ( $X$ ). As it gets darker out, the count might be more variable

# Weighted Regression: Estimating the Weights

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Sometimes there is reason to believe there is unequal variance, but the how the variance is different is unknown

A well used, but utterly heuristic, method is to:

1. fit an ordinary least squares model
2. Get the squared residuals out:  $res_i^2$

It is tempting to use  $w_i = res_i^2$ , (as the residuals estimate the noise term  $\varepsilon$ )

However, usually the residuals are too noisy to work directly

**Instead:** run another regression, using  $res_i^2$  as the “response”

The “explanatory variable” will be different, depending on the nature of the heteroscedasticity

# Weighted Regression: Estimating the Weights

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A rough guide on how to regress the  $res_i^2$  to estimate the  $w_i$

**Residual plot vs.  $x_j$  has “funnel shape”:** Regress  $|res_i|$  against  $x_j$ . The resulting fitted values of this regression are estimates of  $\sigma_i$ , hence set  $w_i$  to the reciprocal squared

**Residual plot vs.  $\hat{\mu}\{Y_i|X_i\}$  has a “funnel shape”:** Regress  $|res_i|$  against  $\hat{\mu}\{Y_i|X_i\}$ . The resulting fitted values of this regression are estimates of  $\sigma_i$ , hence set  $w_i$  to the reciprocal squared

**Plot of  $res_i^2$  vs.  $x_j$  has a trend:** Regress  $res_i^2$  against  $x_j$ . The resulting fitted values of this regression are estimates of  $\sigma_i^2$ , hence set  $w_i$  to the reciprocal

**Plot of  $res_i^2$  vs.  $\hat{\mu}\{Y_i|X_i\}$  has a trend:** Regress  $res_i^2$  against  $\hat{\mu}\{Y_i|X_i\}$ . The resulting fitted values of this regression are estimates of  $\sigma_i^2$ , hence set  $w_i$  to the reciprocal

# Nonlinear Regression

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# Returning to Kleiber's Law

```
DATA mammal;
INPUT CommonName $ Species $ Mass Metab Life;
DATALINES;
Echidna Tachiglossus_aculeatus 2.500 302.00 14
Long-beaked_echidna Zaglossus_bruijnii 10.300 594.00 20
Platypus Ornithorhynchus_anatinus 1.300 229.00 9
Opossum Lutreolina_crassicaudata 0.812 196.00 5
South_American_opossum Didelphis_marsupialis 1.330 299.00 6
Virginia_opossum Didelphis_virginiana 3.260 519.00 8
Australian_marsupial Antechinus_macdonnellensis 0.014 9.00 2
Marsupial Antechinus_stuartii 0.004 17.60 2.5
Marsupial Antechinus_laniger 0.009 5.17 2
Marsupial_rat Dasyuroides_byrnei 0.089 37.40 3
Bandicoot Isodon_macrodonatus 1.000 201.00 8
Long-nosed_bandicoot Perameles_nasuta 0.645 153.00 7
Fat-tailed_dunnart Sminthopsis_crassicaudata 0.015 9.64 2
Australian_marsupial Planigale_maculata 0.013 13.70 1.5
Tasmanian_devil Sacrophilus_harrisii 5.050 628.00 10
Brush-tail_possum Trichosurus_vulpecula 1.980 306.00 8
Kangaroo Macropus_robustus 4.690 694.00 11
Red_kangaroo Macropus_rufus 40.000 4000.00 15
Tamar wallaby Macropus_eugenii 4.800 671.00 11
Sloth Bradypus_variegatus 3.790 331.00 19
Armadillo Dasypus_noveboracensis 3.320 384.00 10
Pangolin Manis_triensis 2.730 440.00 8
```

**Kleiber's Law:**  $\text{metabolism} \propto \text{mass}^{3/4}$

Let's directly estimate this model via nonlinear regression

(Note: we are looking at metabolism as the response, mass as explanatory variable)



# Nonlinear Regression

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The linear regression model is  $Y_i = \beta_0 + \sum_{j=1}^p X_{ij}\beta_j + \varepsilon_i$

which gets estimated via least squares as

minimize  $\sum_{i=1}^n (Y_i - (\beta_0 + \sum_{j=1}^p X_{ij}\beta_j))^2$

Nonlinear Regression is similar, it is just we have a nonlinear model for the mean,  $Y_i = \mu\{Y_i|X_i\} + \varepsilon_i$

which still gets estimated via least squares as

minimize  $\sum_{i=1}^n (Y_i - \mu\{Y_i|X_i\})^2$ ,

where the minimization is over the parameters in the model  $\mu\{Y_i|X_i\}$

# Kleiber's Law as a Nonlinear Regression

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$$Y_i = \mu\{Y_i|X_i\} + \varepsilon_i = \beta_0 + \sum_{j=1}^p X_i \beta_j + \varepsilon_i$$

$$Y_i = \mu\{Y_i|X_i\} + \varepsilon_i = \beta_0 X_i^{\beta_1} + \varepsilon_i$$

**Kleiber's Law** posits that  $\beta_1 = 3/4$  but it leaves  $\beta_0$  unspecified

We can estimate this model in two ways, but they aren't equivalent

- $\log(\beta_0 X_i^{\beta_1}) = \log(\beta_0) + \beta_1 X_i \rightarrow$  Attempt MLR:

$$\log(Y_i) = \log(\beta_0) + \beta_1 X_i + \varepsilon_i$$

“log Y has linear mean with normal errors”

(We can test the “slope” of this model using MLR:  $H_0: \beta_1 = 3/4$ )

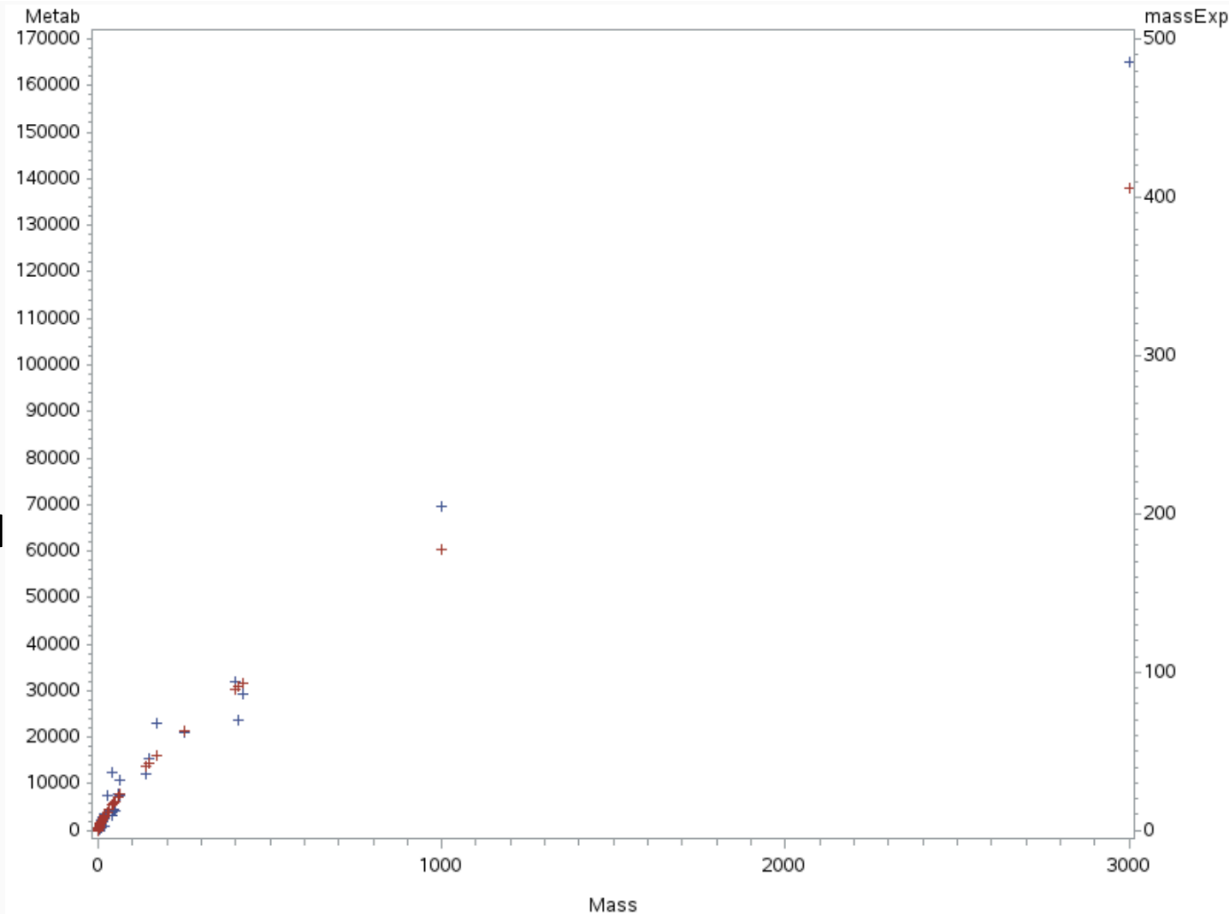
- Or, we can directly fit the nonlinear model:

$$Y_i = \mu\{Y_i|X_i\} + \varepsilon_i = \beta_0 X_i^{\beta_1} + \varepsilon_i$$

“Y has nonlinear mean with normal errors”

# Kleiber's Law as a Nonlinear Regression

```
DATA mammal;  
  SET mammal;  
  massExp = mass**(3/4);  
;  
  
proc gplot data = mammal;  
  plot metab*mass;  
  plot2 massExp*mass;
```



Note the scales of metabolism and massExp have different scales

There is some indication that this particular model is reasonable

# Nonlinear Regression

```
PROC NLIN PLOTS=ALL BEST=10;  
  PARMS  
    theta0=100 to 500 by 10  
    theta1=0 to 1 by 0.01;  
  MODEL metab=theta0*mass**(theta1);  
  OUTPUT out=fitted predicted=yhat;  
RUN;
```

Nonlinear regressions do not necessarily have unique solutions and must be solved iteratively

Hence, the better starting values/grid you can provide, the better chance that you find a good solution

The NLIN Procedure  
Dependent Variable Metab

Grid Search		
theta0	theta1	Sum of Squares
250.0	0.8100	2.5327E8
230.0	0.8200	2.5399E8
270.0	0.8000	2.6078E8
200.0	0.8400	2.616E8
220.0	0.8300	2.7191E8
290.0	0.7900	2.7448E8
210.0	0.8300	2.7465E8
170.0	0.8600	2.9143E8
240.0	0.8200	2.9248E8
180.0	0.8500	2.975E8

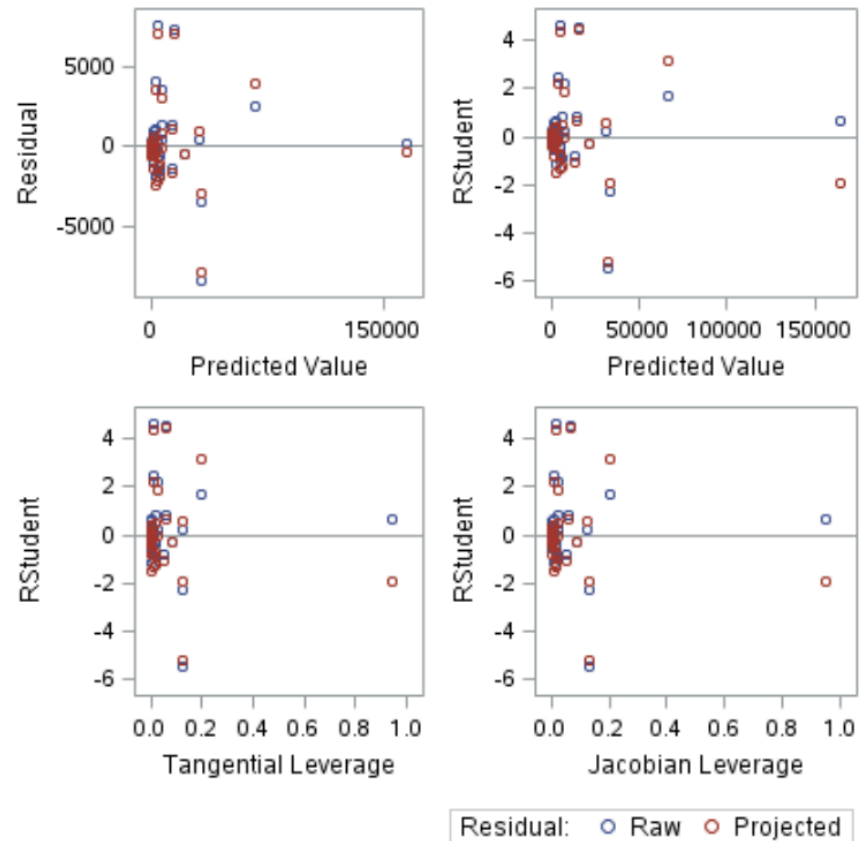
# Nonlinear Regression

```
PROC NLIN PLOTS=ALL BEST=10;  
  PARMS  
    theta0=100 to 500 by 10  
    theta1=0 to 1 by 0.01;  
  MODEL metab=theta0*mass**(theta1);  
  OUTPUT out=fitted predicted=yhat;  
RUN;
```

We can still look at residuals/leverage

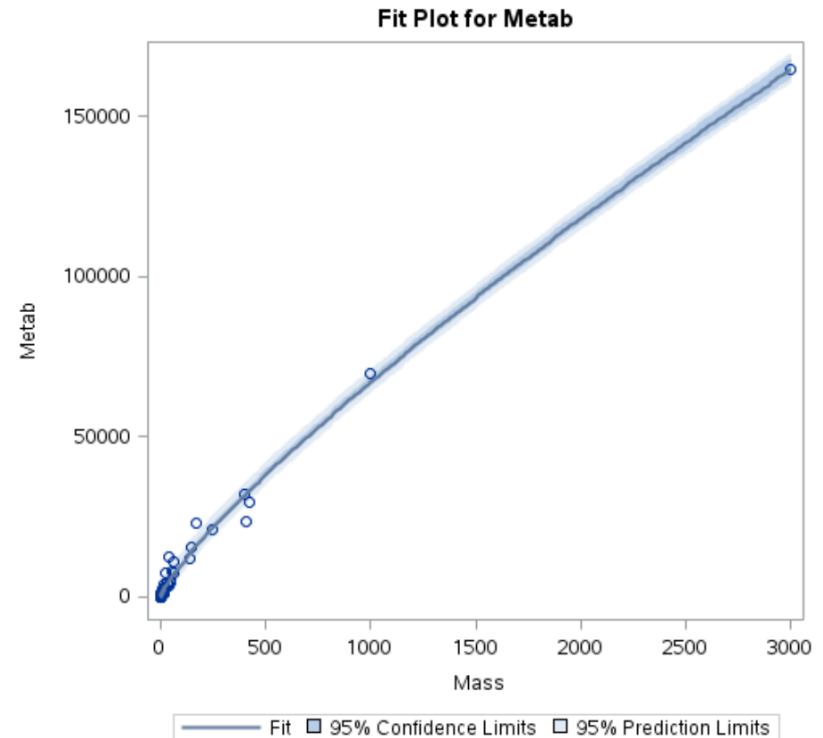
There are more types of each, however

Here, we see at least one high leverage point and some mildly large studentized residuals



# Nonlinear Regression

```
PROC NLIN PLOTS=ALL BEST=10;  
  PARMS  
    theta0=100 to 500 by 10  
    theta1=0 to 1 by 0.01;  
  MODEL metab=theta0*mass**(theta1);  
  OUTPUT out=fitted predicted=yhat;  
RUN;
```

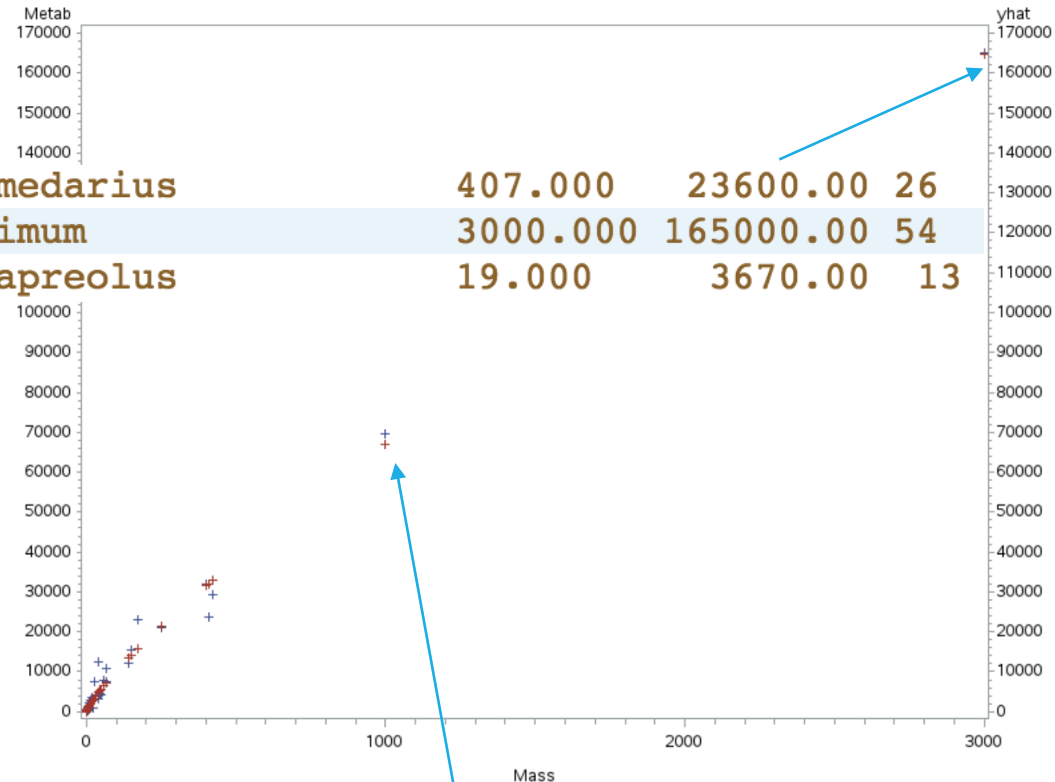


Parameter	Estimate	Approx Std Error	Approximate 95% Confidence Limits	
theta0	233.2	18.1122	197.3	269.2
theta1	0.8194	0.0102	0.7991	0.8396

# Nonlinear Regression

```
proc gplot data = fitted;
plot metab*mass;
plot2 yhat*mass;
```

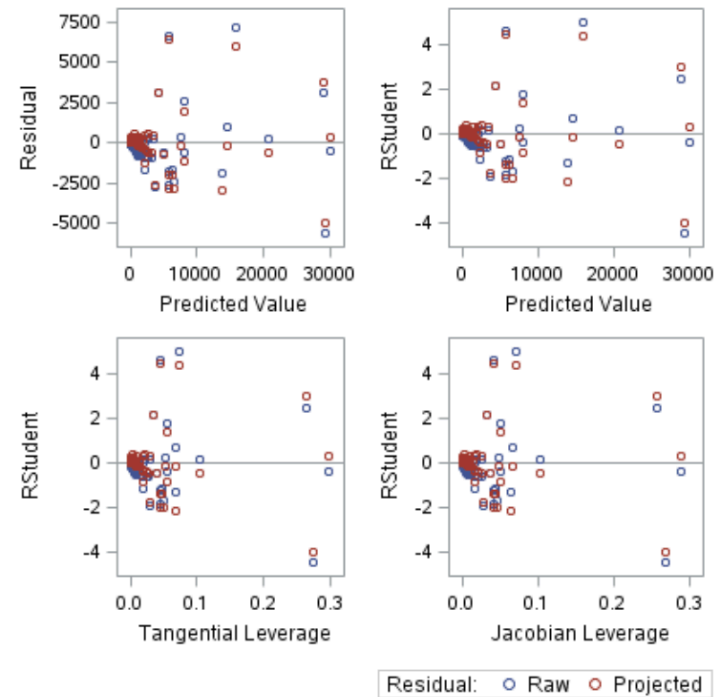
Camel	Camelus_dromedarius	407.000	23600.00	26
Asian_elephant	Elephas_maximum	3000.000	165000.00	54
Roe_deer	Capreolus_capreolus	19.000	3670.00	13



Beluga_whale	Delphinapterus_leucas	170.000	23000.00	25
Bottle-nosed_whale	Hyperoodon_ampullatus	1000.000	69500.00	40
Bat	Desmodus_rotundus	0.029	9.65	8

# Nonlinear Regression: Limiting the Population

```
PROC NLIN PLOTS=ALL BEST=10;  
  WHERE mass<500;  
  PARMS  
    theta0=100 to 500 by 10  
    theta1=0 to 1 by 0.01;  
  MODEL metab=theta0*mass**(theta1);  
  OUTPUT out=fitted predicted=yhat;  
RUN;
```



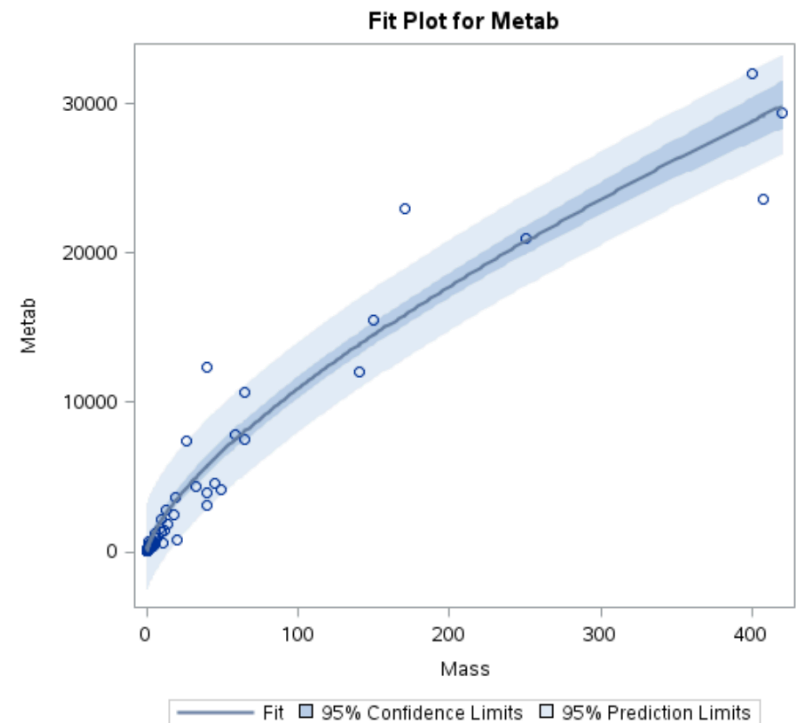


# Nonlinear Regression: Limiting the Population

```
PROC NLIN PLOTS=ALL BEST=10;  
  WHERE mass<500;  
  PARMS  
    theta0=100 to 500 by 10  
    theta1=0 to 1 by 0.01;  
  MODEL metab=theta0*mass**(theta1);  
  OUTPUT out=fitted predicted=yhat;  
RUN;
```

Conclusion: there is no evidence against the Kleiber's Law hypothesized value

Also, we get an estimate for the proportionality constant: 437.5



Parameter	Estimate	Approx Std Error	Approximate 95% Confidence Limits	
theta0	437.5	65.5825	307.2	567.8
theta1	0.6992	0.0269	0.6459	0.7526

# Nonlinear Regression: Limiting the Population

```
PROC NLIN PLOTS=ALL BEST=10;  
  WHERE mass<500;  
  PARMS  
    theta0=100 to 500 by 10  
    theta1=0 to 1 by 0.01;  
  MODEL metab=theta0*mass**(theta1);  
  OUTPUT out=fitted predicted=yhat;  
RUN;
```

```
proc gplot data = fitted;  
  plot metab*mass;  
  plot2 yhat*mass;
```

