Multiple Regression: A Model for the Mean

STRUCTURAL VS. DATA-BASED MULTICOLLINEARITY
WEIGHTED REGRESSION
NONLINEAR REGRESSION

Types of Multicollinearity

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

Data-Based Multicollinearity

The inclusion of additional explanatory variables has several effects

We've talked about some of the benefits:

Possibly improving model fit

- "variance considerations"
- •Decreasing the (estimated) variance s^2
- Controlling for confounders (in an observational study)

"design considerations"

However, there are some definite costs:

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

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

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"

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

Reminder: The variance σ^2 is estimated by $s^2 = MSE$, which can be found on the ANOVA table

Source	DF	Sum of Squares	Mear	Square	F Value	Pr > F
Model	4	3.988723E13	9.971	8076E12	88.94	<.0001
Error	24	2.6908501E12	11211	8754091		
Corrected Total	28	4.257808E13				

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

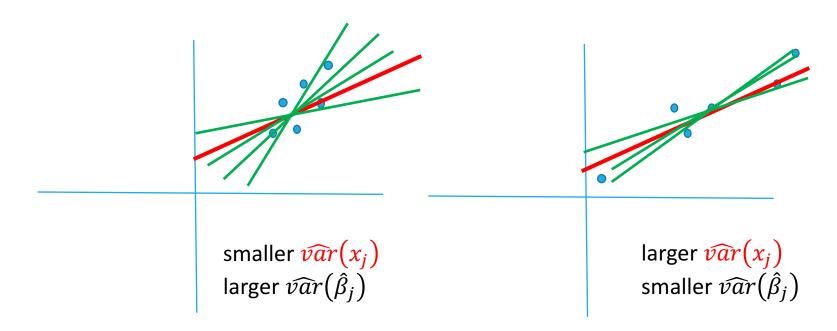
As we add more terms to the model

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

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

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

The variability of the explanatory variable contributes to the variance



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

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

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

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

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

Data-Based Multicollinearity

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- Controlling for confounders (in an observational study)

However, there are some definite costs:

- $ullet \widehat{var}(\hat{eta}_i)$ tends to increase as more terms are added
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The "benefits" vs. "costs" depends on the specifics of the explanatory variables

"design considerations"

Design Considerations: Controlling for confounders

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

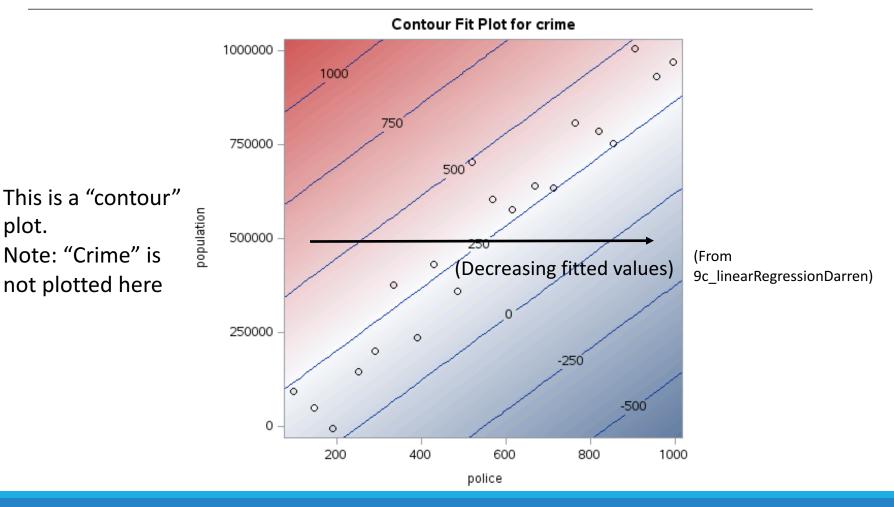
Parameter	Estimate	Standard Error	t Value	Pr > t	
Intercept	121.8850878	63.91254453	1.91	0.0726	
police	0.2735152	0.10408009	2.63	0.0171	

```
PROC GLM DATA = population PLOTS = ALL;
    MODEL crime = police population / SOLUTION;
    9c_linearRegressionDarren)
RUN;
```

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

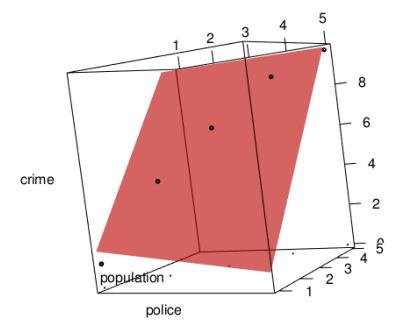
plot.



Go to Visualization...

In-class experiment with code:

 $12a_regression Investigation. R\\$



Design Considerations: Experimental Design

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

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 <u>ORTHOGONAL</u> 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

Suppose we have two explanatory variables x_1 and x_2

If x_1 and x_2 are not orthogonal, then the estimate of β_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 β_1 , β_2 will satisfy this

Design Considerations: Observational Studies

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{eta}_1 will be a large positive number, \hat{eta}_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

3.1 2.9 4

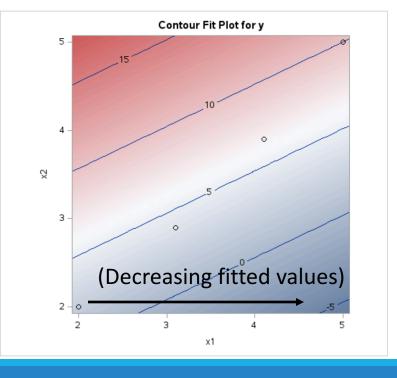
4.1 3.9 6.5

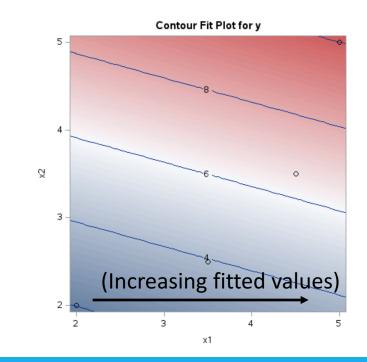
5 5 10
```

DATA mu]	Lti;		
INPU	JT x1	L x2	у;
	DATA	ALINE	S;
	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

Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	-3.275000000	0.19202864	-17.05	0.0373
х1	0.575000000	0.11456439	5.02	0.1252
x2	2.075000000	0.11456439	18.11	0.0351

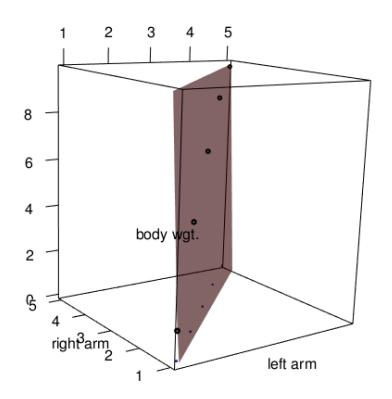




Go to Visualization...

In-class experiment with code:

12a_regressionInvestigation.R



Multicollinearity & Predictions

Back to Decomposing the Prediction Accuracy

•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:

 $Y - \left(\widehat{\beta_0} + \sum_{j=1}^p \widehat{\beta_j} x_j\right) =$ Approximation error + Estimation error + Irreducible Error, where:

- Approximation error: $\mu\{Y|X\} \left(\beta_0 + \sum_{j=1}^p \beta_j x_j\right)$
- Estimation error: $(\beta_0 + \sum_{j=1}^p \beta_j x_j) (\widehat{\beta_0} + \sum_{j=1}^p \widehat{\beta_j} x_j)$
- Irreducible error: ε

Multicollinearity and Predictions

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

$$Y - \left(\widehat{\beta_0} + \sum_{j=1}^p \widehat{\beta_j} x_j\right) =$$
 Approximation error + Estimation error + 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 $\widehat{\mu}$: $(\mathbb{E}\widehat{\mu} \{Y_i|X_i\} - \mu\{Y_i|X_i\})^2 + \mathbb{E}(\widehat{\mu} \{Y_i|X_i\} - \mathbb{E}\widehat{\mu} \{Y_i|X_i\})^2]$
- Irreducible error: ε
- 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

Example: Kleiber's Law

matrix among all the explanatory variables)

```
DATA mammal;
   INPUT CommonName
                      $ Species $
                                                Mass
                                                         Metab
                                                                 Life:
                                                                                                    □proc sqscatter data = mammal;
   DATALINES:
                                                                                                      matrix llife lmetab lmass;
                        Tachiglossus aculeatus
   Echidna
                                                  2.500
                                                         302.00
   Long-beaked echidna
                        Zaglossus bruijni
                                                 10.300
                                                         594.00
                                                                                                      run;
   Platypus
                        Ornithorhynchus anatinus
                                                  1.300
                                                         229.00
   Opossum
                        Lutreolina crassicaudata
                                                  0.812
                                                         196.00
   South American opossu Didelphis marsupialis
                                                         299.00
   Virginia opossum
                        Didelphis virginiana
                                                  3.260
                                                         519.00
   Australian marsupial Antechinus macdonnellensis
                                                  0.014
                                                         9.00
   Marsupial
                        Antechinomus stuartii
                                                  0.004
                                                         17.60
                                                                  2.5
   Marsupial
                        Antechinomus laniger
                                                  0.009
                                                         5.17
                        Dasyuroides_byrnei
   Marsupial rat
                                                  0.089 37.40
   Bandicoot
                        Isodon macroonurus
                                                  1.000
                                                         201.00
   Long-nosed bandicoot Perameles nasuta
                                                  0.645
                                                         153.00
                        Sminthopsis crassicaudata
   Fat-tailed dunnart
                                                         9.64
                                                  0.015
   Australian marsupial
                        Planigale maculata
                                                  0.013
                                                         13.70
   Tasmanian devil
                        Sacrophilus harrisii
                                                  5.050
                                                         628.00
                                                                                                                      Imetab
                        Trichosurus vulpecula
   Brushtail possum
                                                  1.980
                                                         306.00
   Kangaroo
                        Macropus robustus
                                                         694.00
                                                         4000.00
   Red kangaroo
                        Macropus rufus
                                                 40.000
   Tammar wallaby
                        Macropus eugenii
                                                  4.800
                                                         671.00
   Sloth
                        Bradypus variegatus
                                                  3.790
                                                         331.00
                                                                                                                                                    - 7.5
   Armadillo
                        Dasypus novemcinctus
                                                  3.320
                                                         384.00
   Pangolin
                        Manis tricuspis
                                                                                                                                                     5.0
□data mammal:
                                          Kleiber's Law:
                                                                                                                                                    - 2.5
  set mammal;
                                                                                                                                         Imass
 llife = log(life);
                                                                                                                                                     0.0
                                          metabolism ∝ mass<sup>3/4</sup>
 lmetab = log(metab);
                                                                                                                                                     -2.5
 lmass = log(mass);
                                                                                                                                 -5.0 -2.5 0.0 2.5 5.0 7.5
Dproc reg data = mammal;
                                                                                                               Parameter Estimates
  model llife = lmass lmetab / vif;
                                                                                                         Parameter
                                                                                                                    Standard
                                                                                                                                            Variance
                                                                                                                       Error t Value Pr > |t|
                                                                                            Variable DF
                                                                                                          Estimate
                                                                                                                                             Inflation
   run;
                                                                                            Intercept
                                                                                                            4.25340
                                                                                                                     0.52284
                                                                                                                                8.14
                                                                                                                                     <.0001
  (Note: Using PROC CORR you can create the correlation
                                                                                            Imass
                                                                                                            0.61670
                                                                                                                     0.07161
                                                                                                                                8.61
                                                                                                                                     <.0001
                                                                                                                                             34.88426
```

Imetab

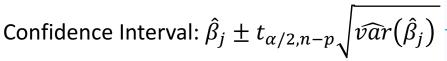
-0.41438

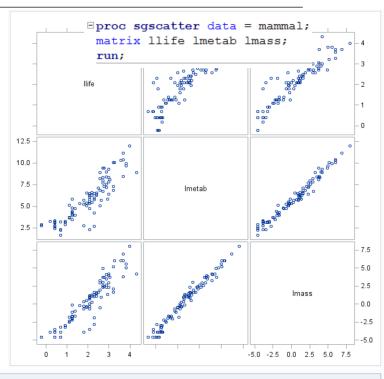
0.09312

34.88426

Confidence Intervals for Coefficients

```
DATA mammal;
    INPUT CommonName
                        $ Species $
                                                  Mass
                                                           Metab
                                                                    Life:
    DATALINES:
                          Tachiglossus aculeatus
                                                           302.00
    Echidna
                                                    2.500
    Long-beaked echidna
                         Zaglossus bruijni
                                                    10.300
                                                           594.00
                         Ornithorhynchus_anatinus
    Platypus
                                                    1.300
                                                           229.00
    Opossum
                         Lutreolina crassicaudata
                                                    0.812
                                                           196.00
    South American opossu Didelphis marsupialis
                                                    1.330
                                                          299.00
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                                                           9.00
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                         Antechinomus stuartii
                                                    0.004
                                                           17.60
                                                                     2.5
    Marsupial
                         Antechinomus laniger
                                                    0.009
                                                            5.17
    Marsupial rat
                         Dasyuroides_byrnei
                                                    0.089 37.40
    Bandicoot
                         Isodon macroonurus
                                                    1.000
                                                           201.00
    Long-nosed bandicoot Perameles nasuta
                                                     0.645
                                                          153.00
                          Sminthopsis crassicaudata
                                                           9.64
    Fat-tailed dunnart
                                                    0.015
    Australian marsupial
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                                                     0.013
                                                           13.70
    Tasmanian devil
                         Sacrophilus harrisii
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                                                           628.00
    Brushtail possum
                         Trichosurus vulpecula
                                                    1.980
                                                           306.00
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                         Macropus robustus
                                                           694.00
    Red kangaroo
                         Macropus rufus
                                                    40.000
                                                           4000.00 15
    Tammar wallaby
                         Macropus eugenii
                                                    4.800
                                                           671.00
    Sloth
                         Bradypus variegatus
                                                    3.790
                                                           331.00
    Armadillo
                         Dasypus novemcinctus
                                                    3.320 384.00
    Pangolin
                         Manis tricuspis
 ∃data mammal:
   set mammal;
  llife = log(life);
  lmetab = log(metab);
  lmass = log(mass);
Dproc reg data = mammal;
 model llife = lmass lmetab / vif clb;
 run;
```





Parameter Estimates									
	Variable	DF	Parameter Estimate		t Value	Pr > t	Variance Inflation	95% Confide	ence Limits
	Intercept	1	4.25340	0.52284	8.14	<.0001	0	3.21468	5.29212
Ī	Imass	1	0.61670	0.07161	8.61	<.0001	34.88426	0.47444	0.75896
	Imetab	1	-0.41438	0.09312	-4.45	<.0001	34.88426	-0.59939	-0.22938

Possible Remediation

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

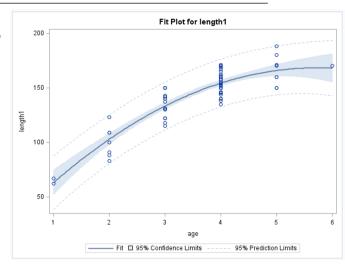
Structural-Based Multicollinearity

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			

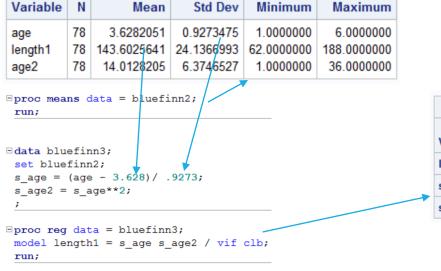
Structural-Based Multicollinearity

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

One solution is via **STANDARDIZATION**

	Parameter Estimates									
Variable	DF	Parameter Estimate		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				

	_				
ĸ	toro	ctan	dard	lizatior	`
	-	SIGII	uaiu	11/011111	



Parameter Estimates										
Variable	DF	Parameter Estimate		t Value	Pr > t	Variance Inflation	95% Confide	ence 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

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 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/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.

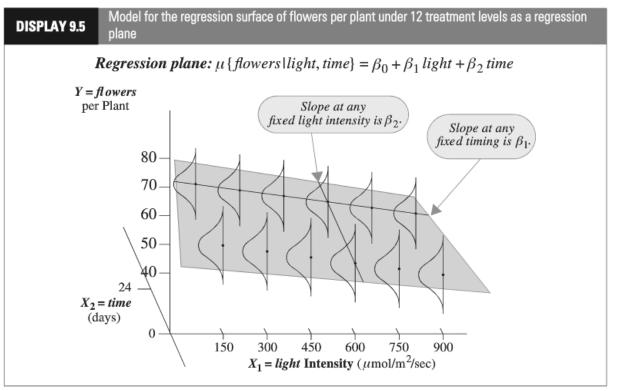
Weighted Regression

Multiple Regression: Constant Variance

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

Regression plane: μ {flowers | light, time} = $\beta_0 + \beta_1$ light + β_2 time

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



"Constant Variance Assumption" (homoscedasticity)

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

Weighted Regression

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:

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 σ_i^2 . Then weighting makes sense

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

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

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 ε)

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

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 σ_i , hence set w_i to the reciprocal squared

Residual plot vs. $\widehat{\mu}\{Y_i|X_i\}$ has a "funnel shape": Regress $|res_i|$ against $\widehat{\mu}\{Y_i|X_i\}$. The resulting fitted values of this regression are estimates of σ_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 σ_i^2 , hence set w_i to the reciprocal

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

Returning to Kleiber's Law

DAT	A mammal;				
	INPUT CommonName \$	Species \$	Mass	Metab	Life;
	DATALINES;				
	Echidna	Tachiglossus_aculeatus	2.500	302.00	14
	Long-beaked_echidna	Zaglossus_bruijni	10.300	594.00	20
	Platypus	Ornithorhynchus_anatinus	1.300	229.00	9
	Opossum	Lutreolina_crassicaudata	0.812	196.00	5
	South_American_opossu	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
	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

Kleiber's Law: metabolism \propto 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)

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

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

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

Kleiber's Law posits that $\beta_1 = 3/4$ but it leaves β_0 unspecified

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

•
$$\log(\beta_0 X_i^{\beta_1}) = \log(\beta_0) + \beta_1 X_i \to \text{Attempt MLR}$$
:

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

"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"

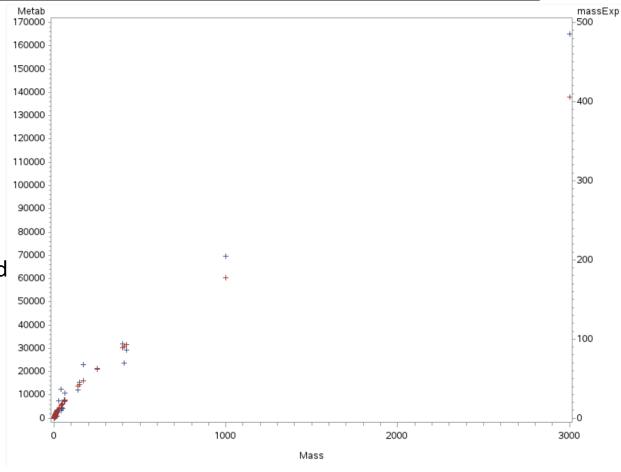
Kleiber's Law as a Nonlinear Regression

```
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



```
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				
I	theta0	theta1	Sum of Squares		
	250.0	0.8100	2.5327E8		
I	230.0	0.8200	2.5399E8		
	270.0	0.8000	2.6078E8		
	200.0	0.8400	2.616E8		
l	220.0	0.8300	2.7191E8		
l	290.0	0.7900	2.7448E8		
l	210.0	0.8300	2.7465E8		
l	170.0	0.8600	2.9143E8		
l	240.0	0.8200	2.9248E8		
1	180.0	0.8500	2.975E8		

```
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);

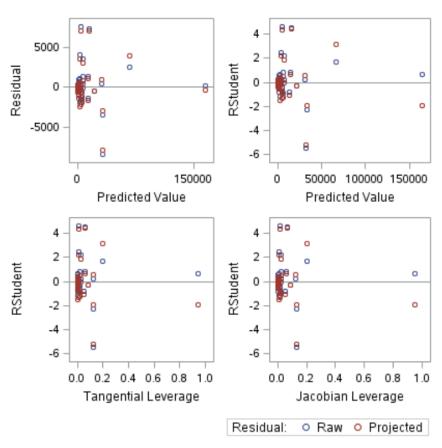
OUTPUT out=fitted predicted=yhat;

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



```
PROC NLIN PLOTS=ALL BEST=10;

PARMS

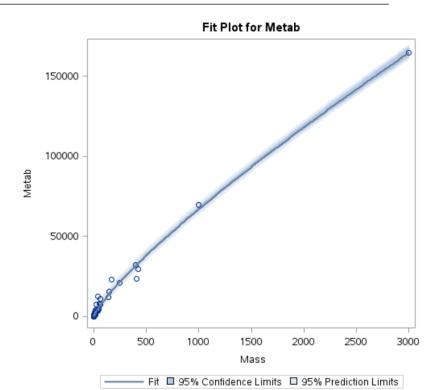
theta0=100 to 500 by 10

theta1=0 to 1 by 0.01;

MODEL metab=theta0*mass**(theta1);

OUTPUT out=fitted predicted=yhat;

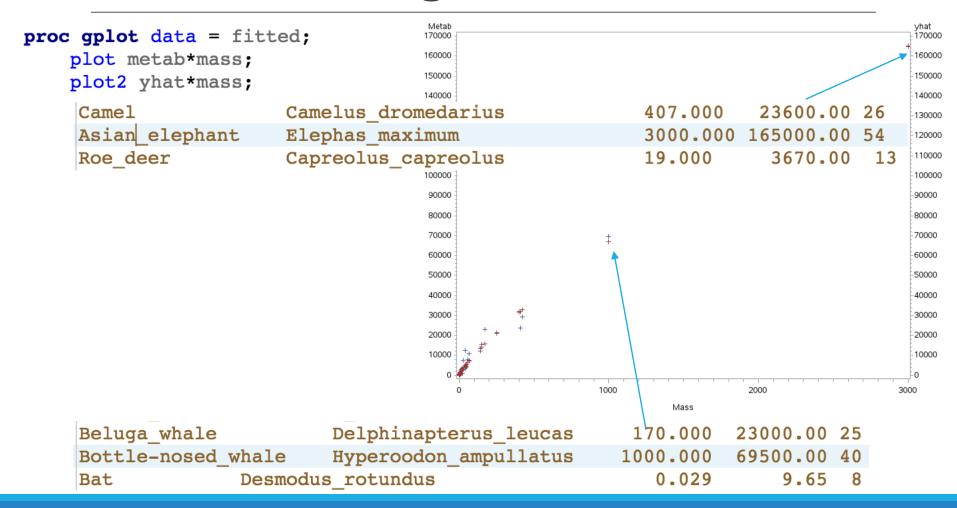
RUN;
```



 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: Limiting the Population

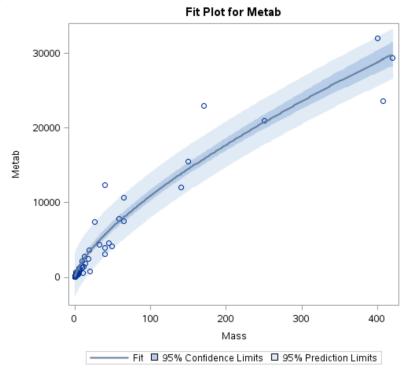
```
PROC NLIN PLOTS=ALL BEST=10;
      WHERE mass<500;
                                                                  7500
      PARMS
                                                                  5000
                                                               Residual
      theta0=100 to 500 by 10
                                                                                        RStudent
                                                                  2500
      theta1=0 to 1 by 0.01;
                                                                  -2500
      MODEL metab=theta0*mass**(theta1);
                                                                 -5000
      OUTPUT out=fitted predicted=yhat;
                                                                         10000 20000 30000
                                                                                                 10000
                                                                                                     20000
                                                                                                           30000
RUN;
                                                                         Predicted Value
                                                                                                 Predicted Value
                                                                                        RStudent
                                                               RStudent
                                                                          0.1
                                                                               0.2
                                                                                   0.3
                                                                                            0.0
                                                                                                  0.1
                                                                                                       0.2
                                                                                                            0.3
                                                                       Tangential Leverage
                                                                                               Jacobian Leverage
                                                                                        Residual: O Raw O Projected
```

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;</pre>
```

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;
                                       30000
                                                                                   30000
proc gplot data = fitted;
    plot metab*mass;
    plot2 yhat*mass;
                                       20000
                                                                                   20000
                                       10000
                                                             Mass
```