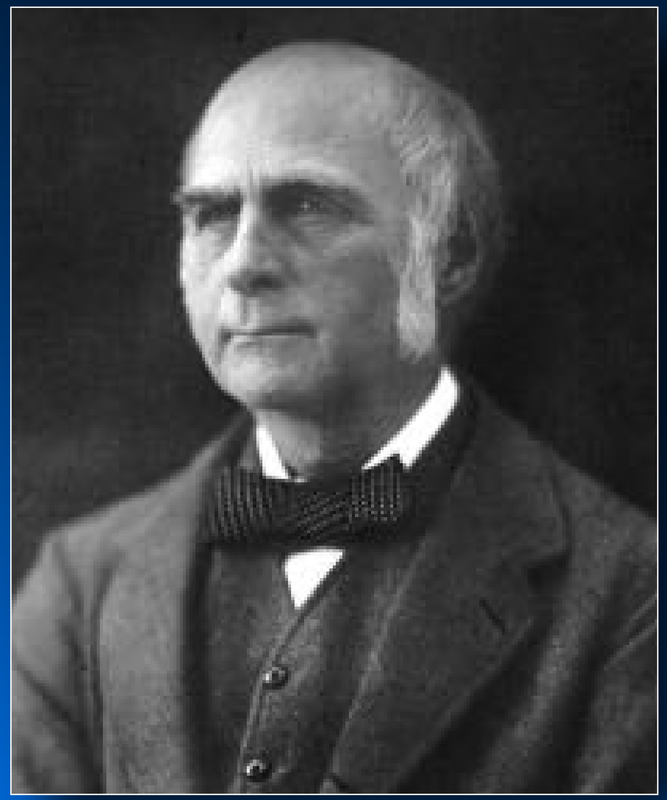
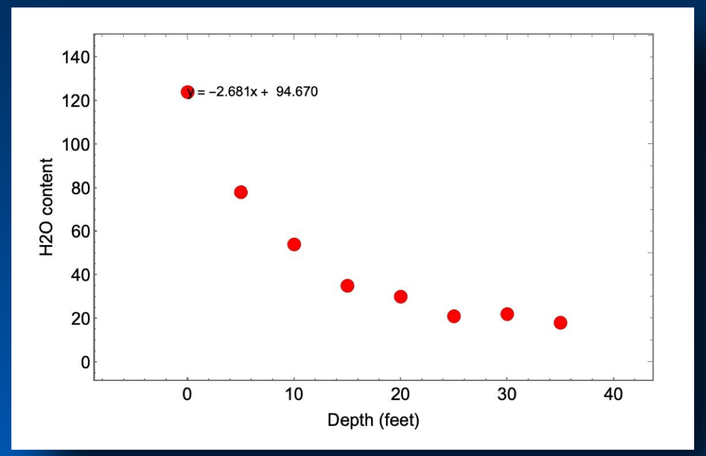
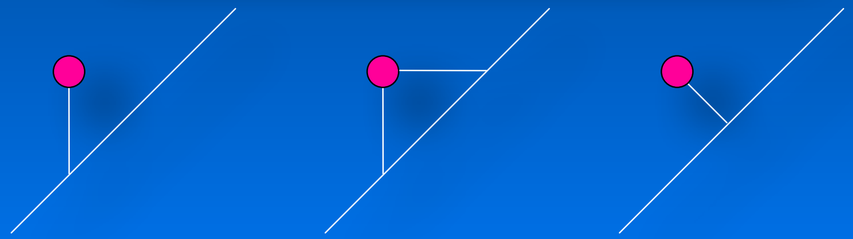
Bivariate Regression, Modeling & Testing of Earth Science Data



Prof. Norman MacLeod

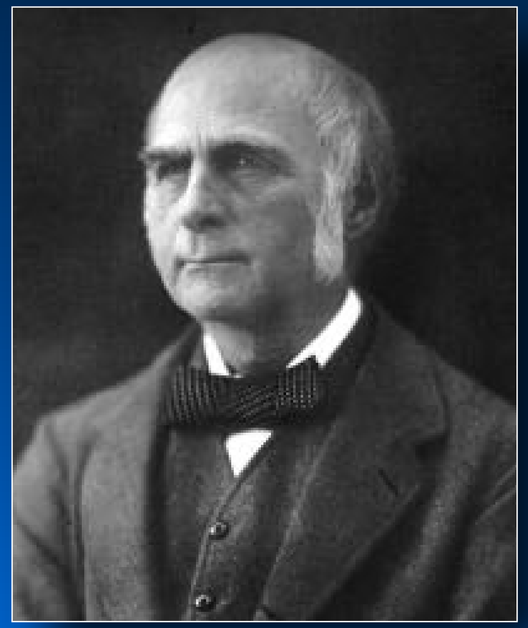
School of Earth Sciences & Engineering, Nanjing University



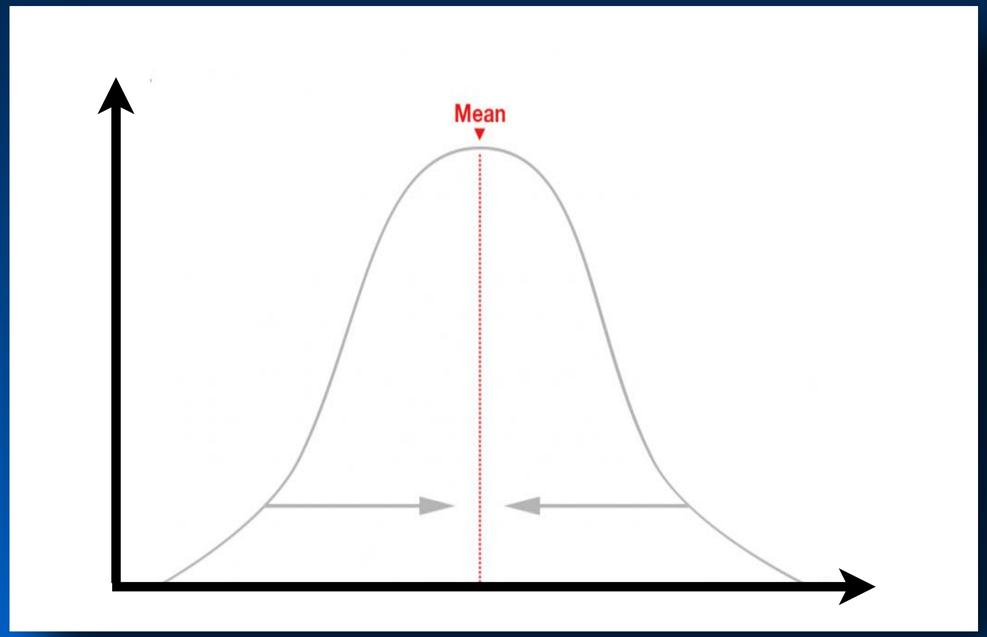


Linear Regression, Modeling & Testing

Regression Analysis - The quantitative study of the manner in which variation in one (or more) variable(s) can be expressed in terms of variation in one (or more) other variable(s).



Francis Galton
(1822 - 1911)



Regression to the Mean

Developed originally by Galton to model heritability of physical dimensions between parents and children; a critical early demonstration of Darwin's principle of biological heredity.

Linear Regression, Modeling & Testing

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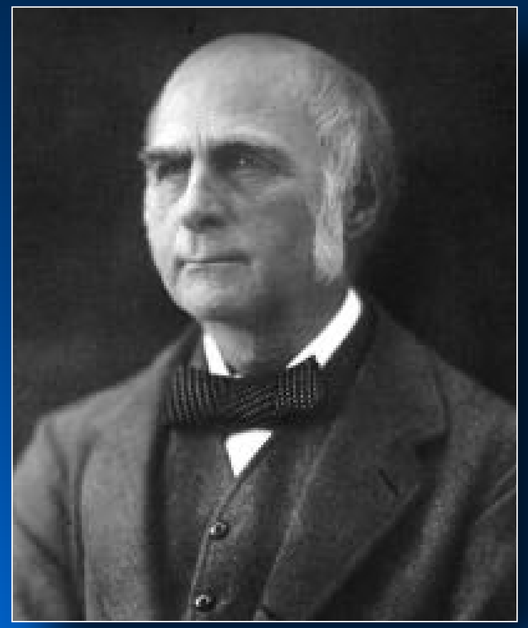

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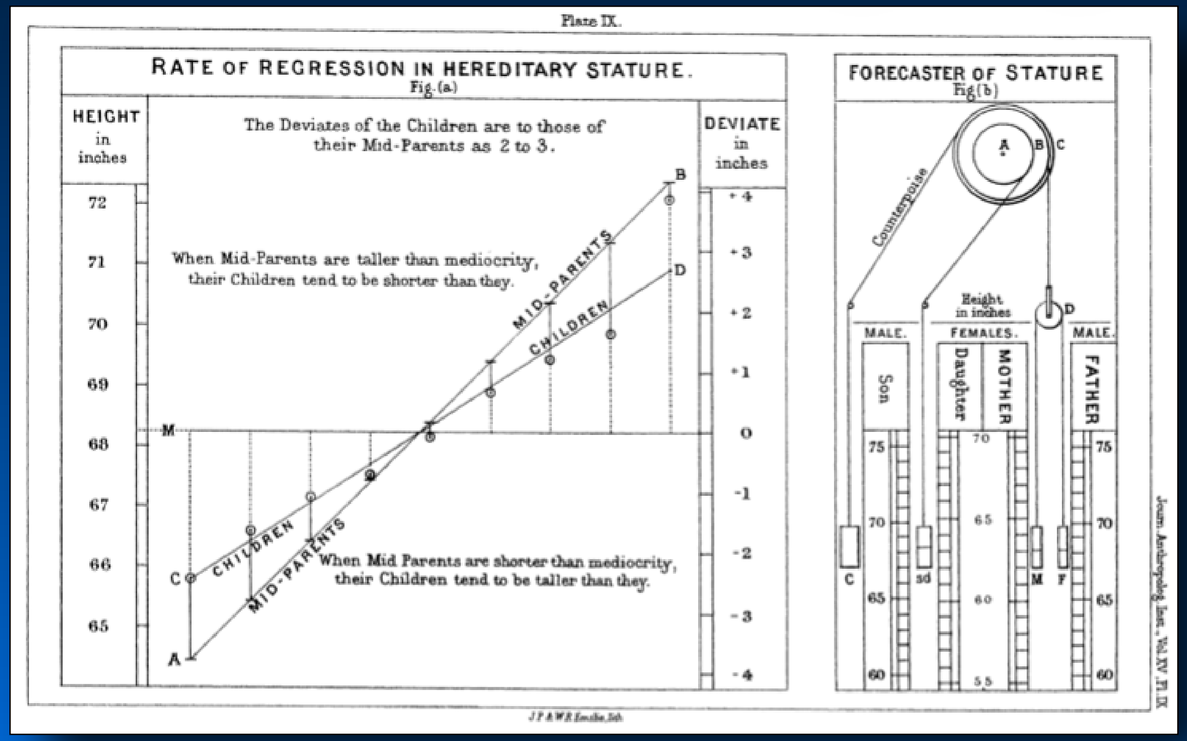

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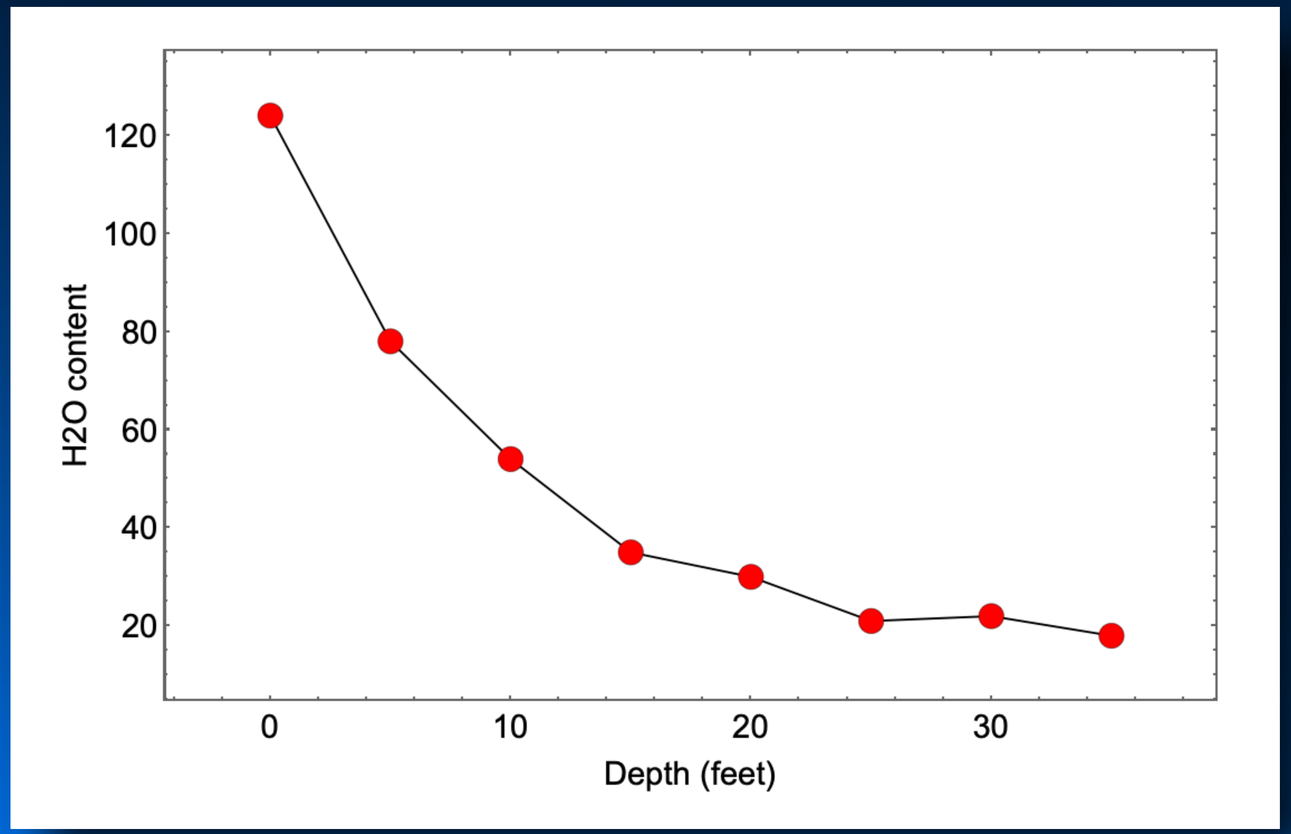
Linear Regression, Modeling & Testing

Depth vs H_20 Content of Louisiana Estuary Mud

Depth (Feet)	H_20 Content (g/100g solids)
0	124
5	78
10	54
15	35
20	30
25	21
30	22
35	18



Obviously water content diminishes with depth, probably due to weight compaction. But can we model this relationship quantitatively and test its conformance to a strictly linear model?

Linear Regression, Modeling & Testing

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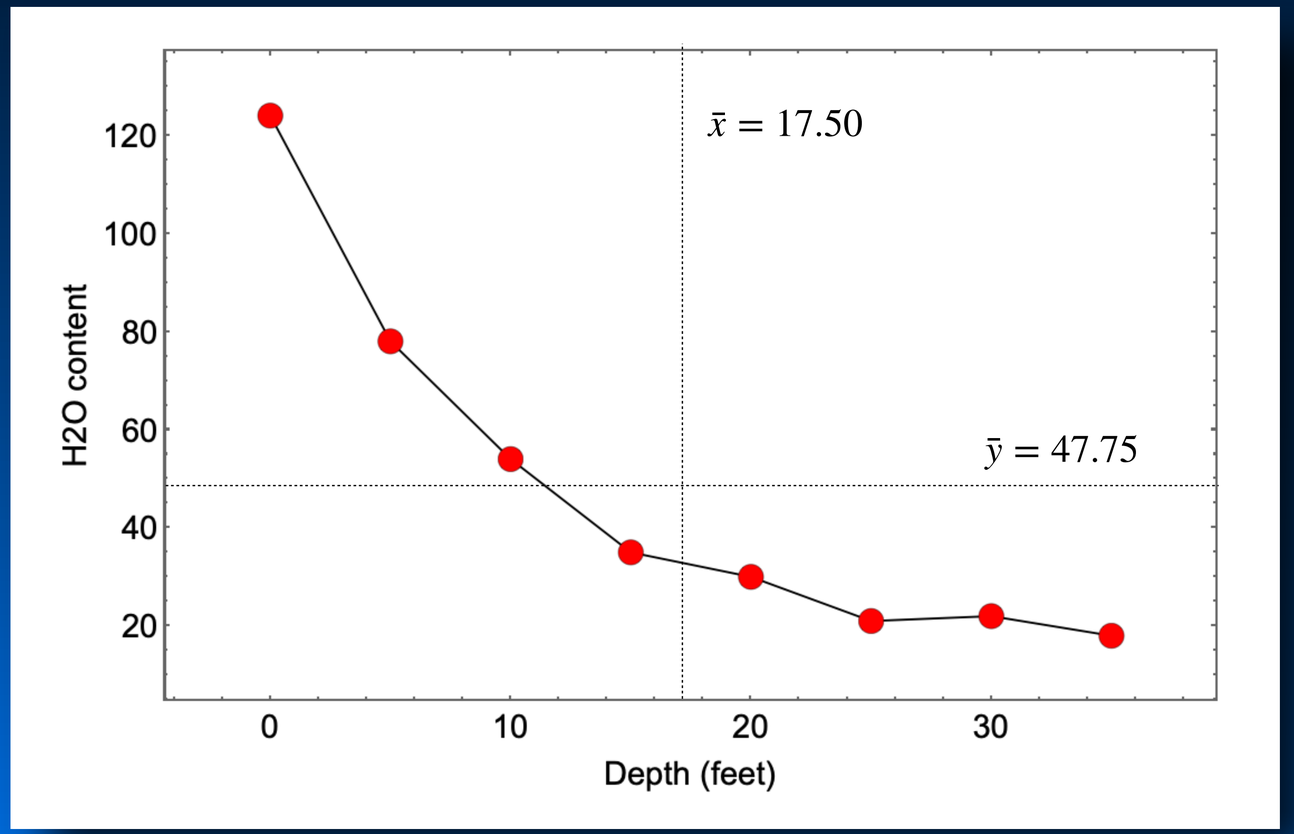

The first thing we might want to do is find a fixed point in the data. Since the arithmetic mean is a parameter we can use to locate the variable distributions relative to one another, that's a logical choice.

Linear Regression, Modeling & Testing

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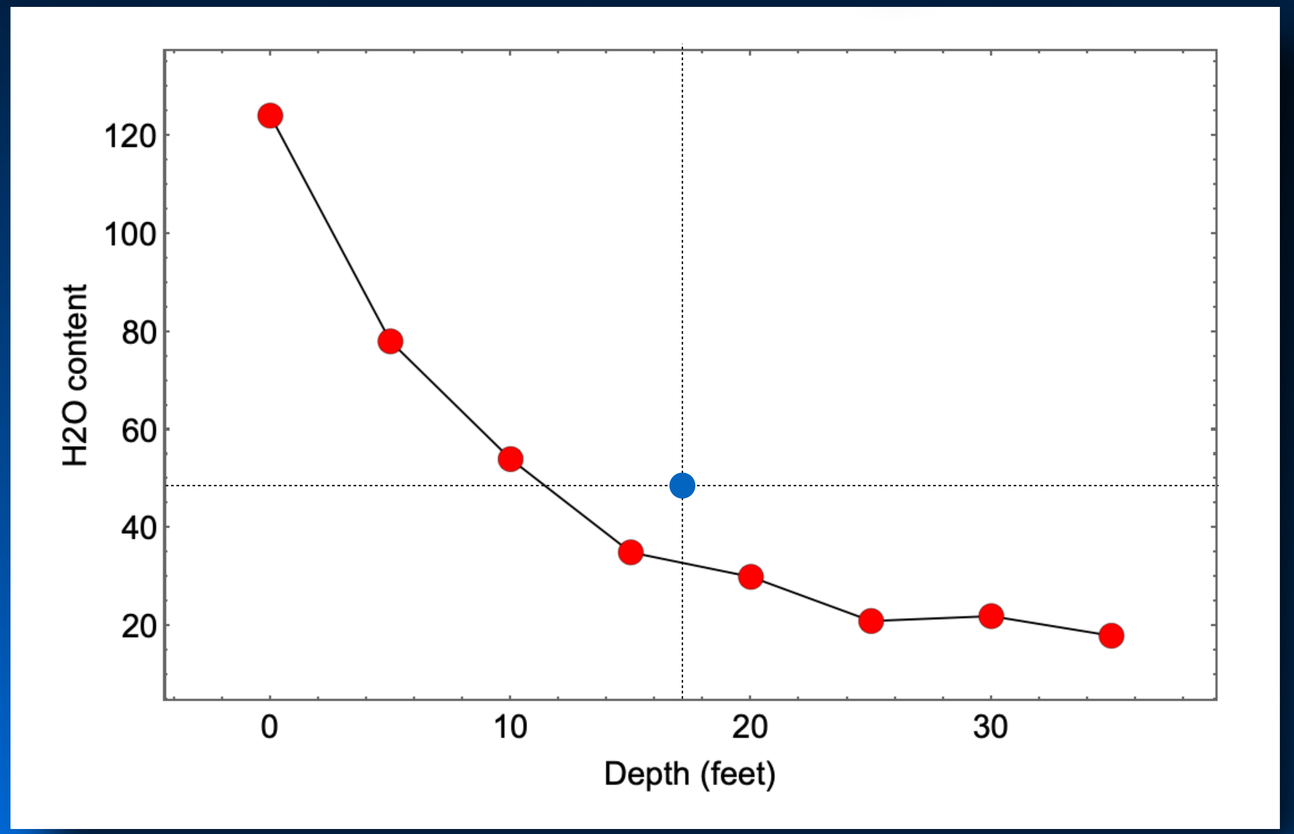

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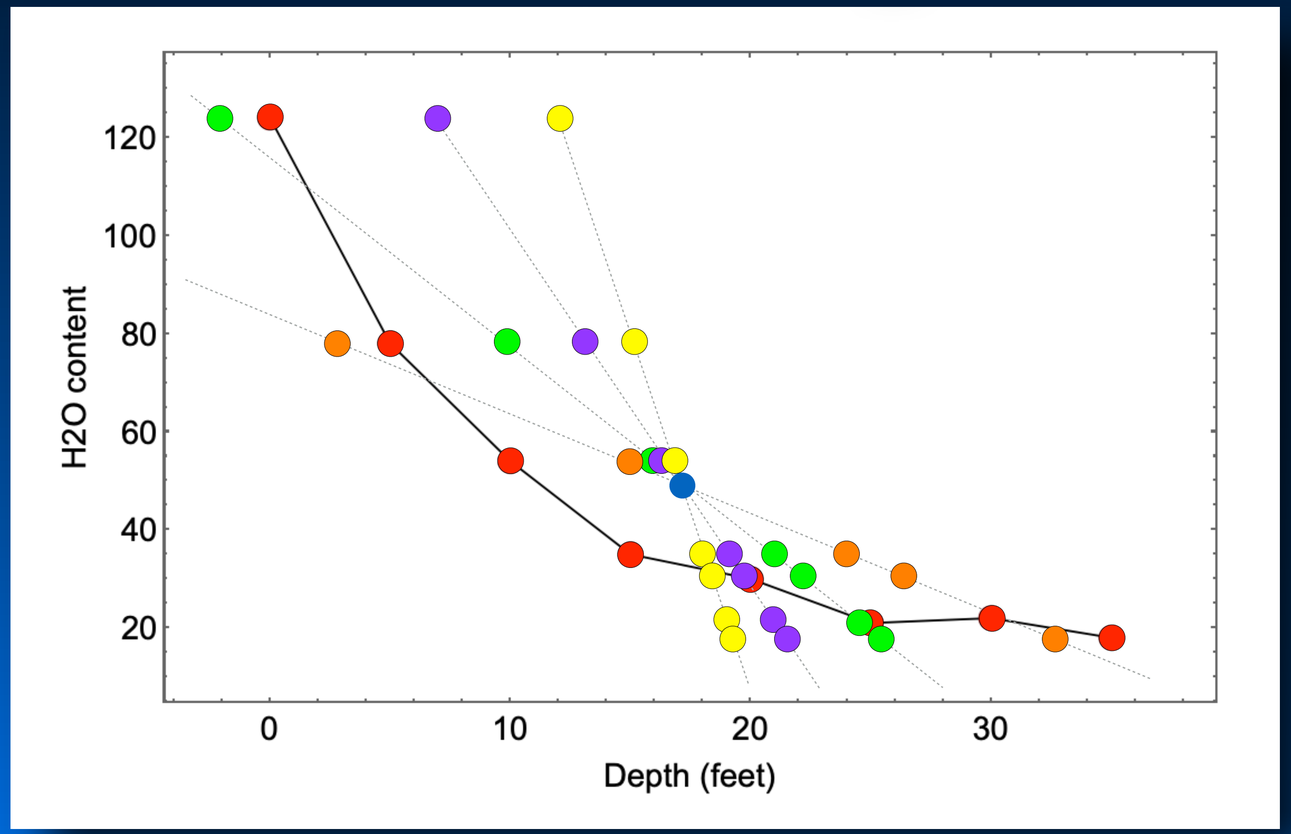

What we want is a straight line (=model) that minimizes its deviation from the data. We can find this by trial & error, and actually, this strategy has begun to be advocated.

Linear Regression, Modeling & Testing

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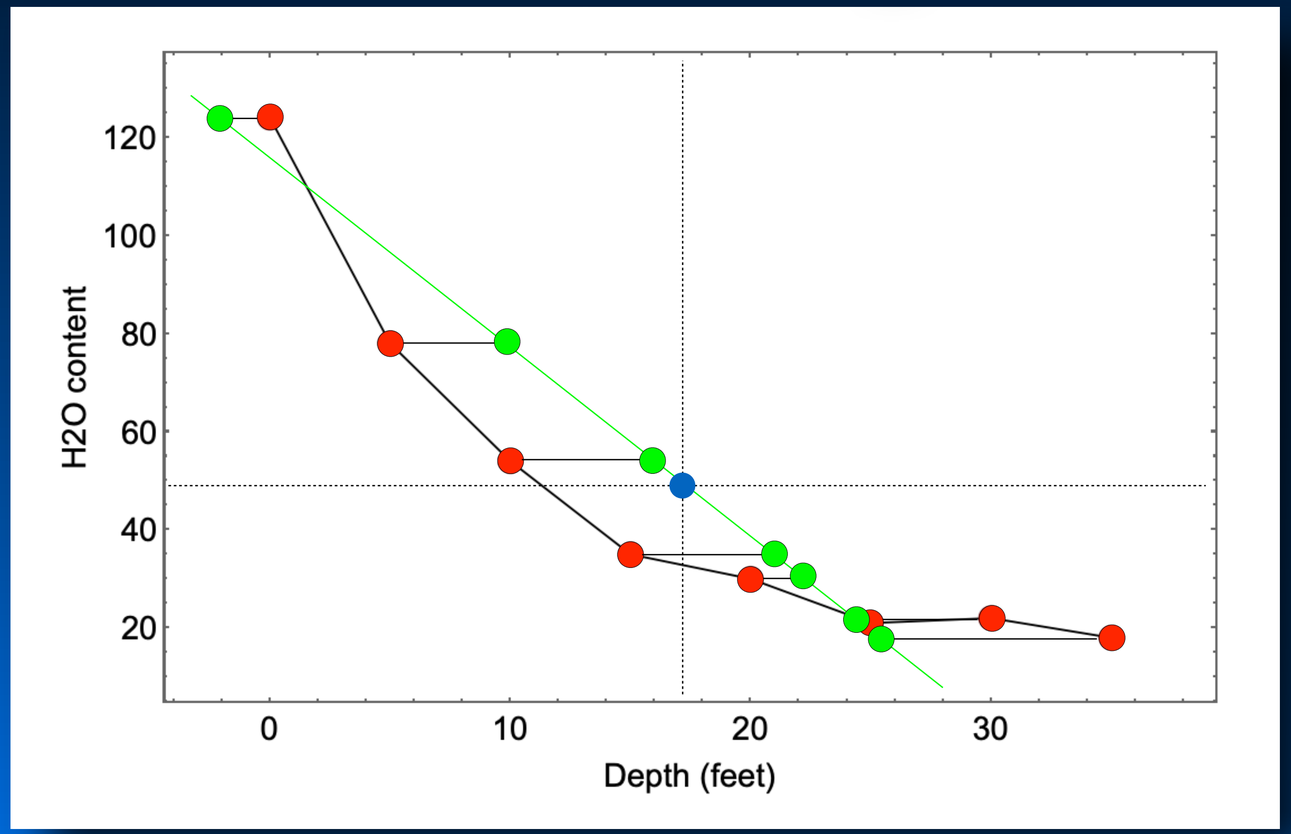

This model minimizes error in the x-value. It's called an "y on x" regression and it should be used when you want to estimate the values of x when you know the values of y.

Linear Regression, Modeling & Testing

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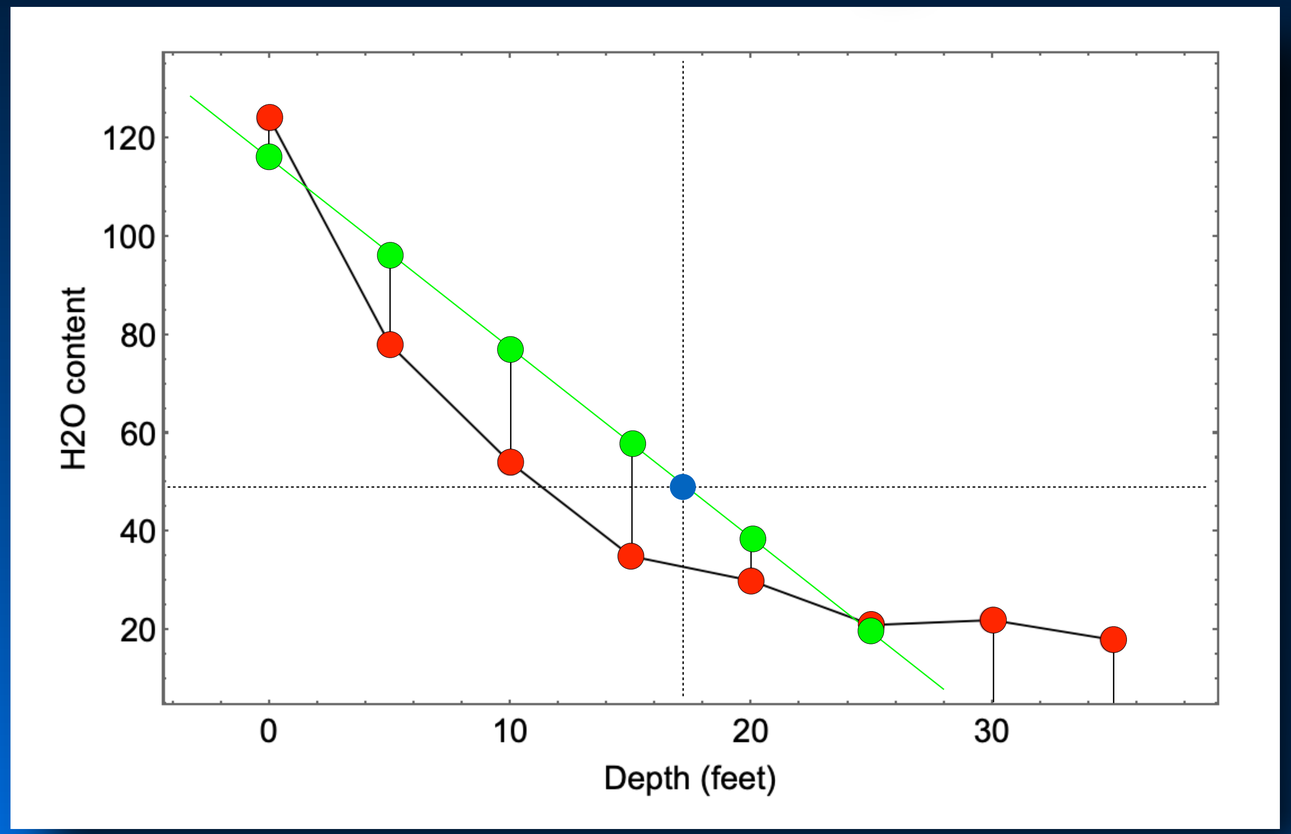

But this model doesn't seem to fit the data in the y direction very well.

Linear Regression, Modeling & Testing

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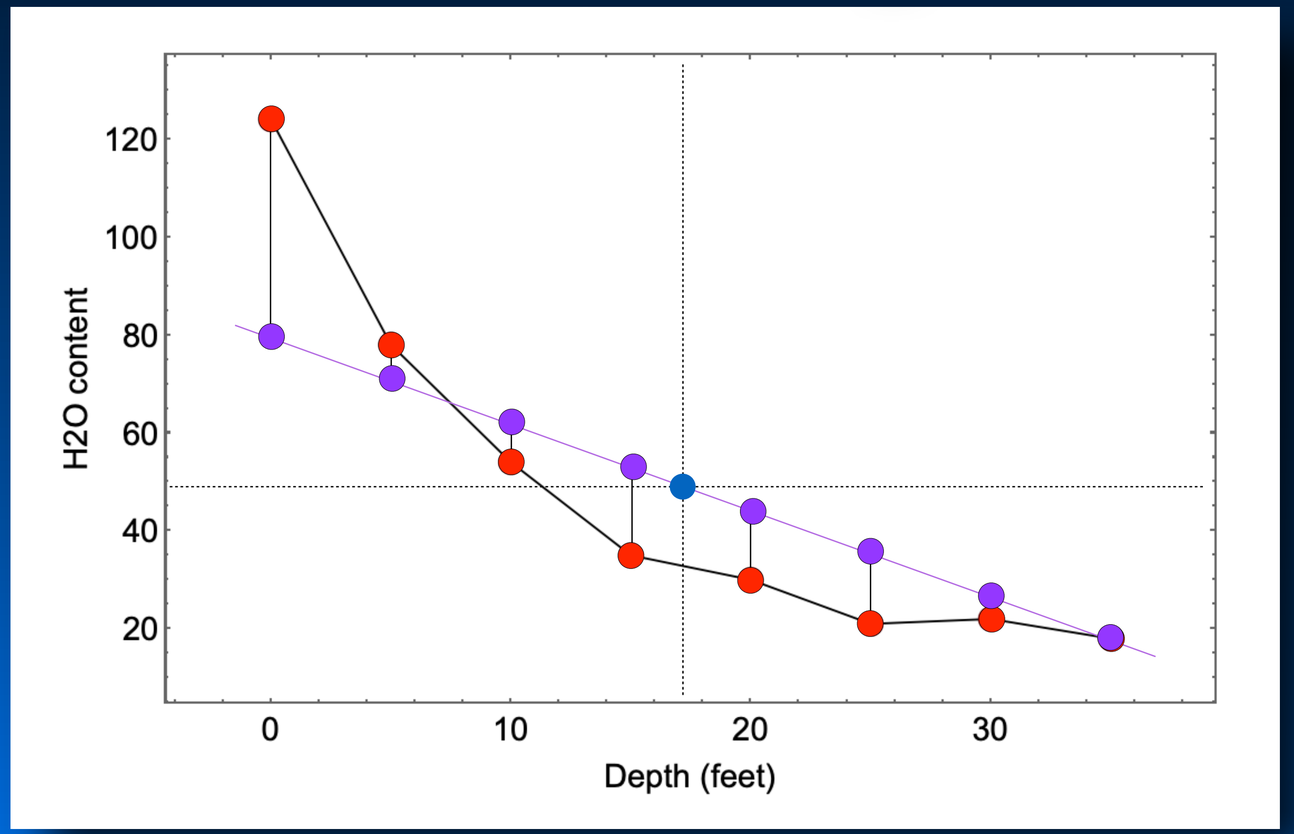

This model minimizes error in the y-value. It's called an "x on y" regres-sion and it should be used when you want to estimate the values of y when you know the values of x.

Linear Regression, Modeling & Testing

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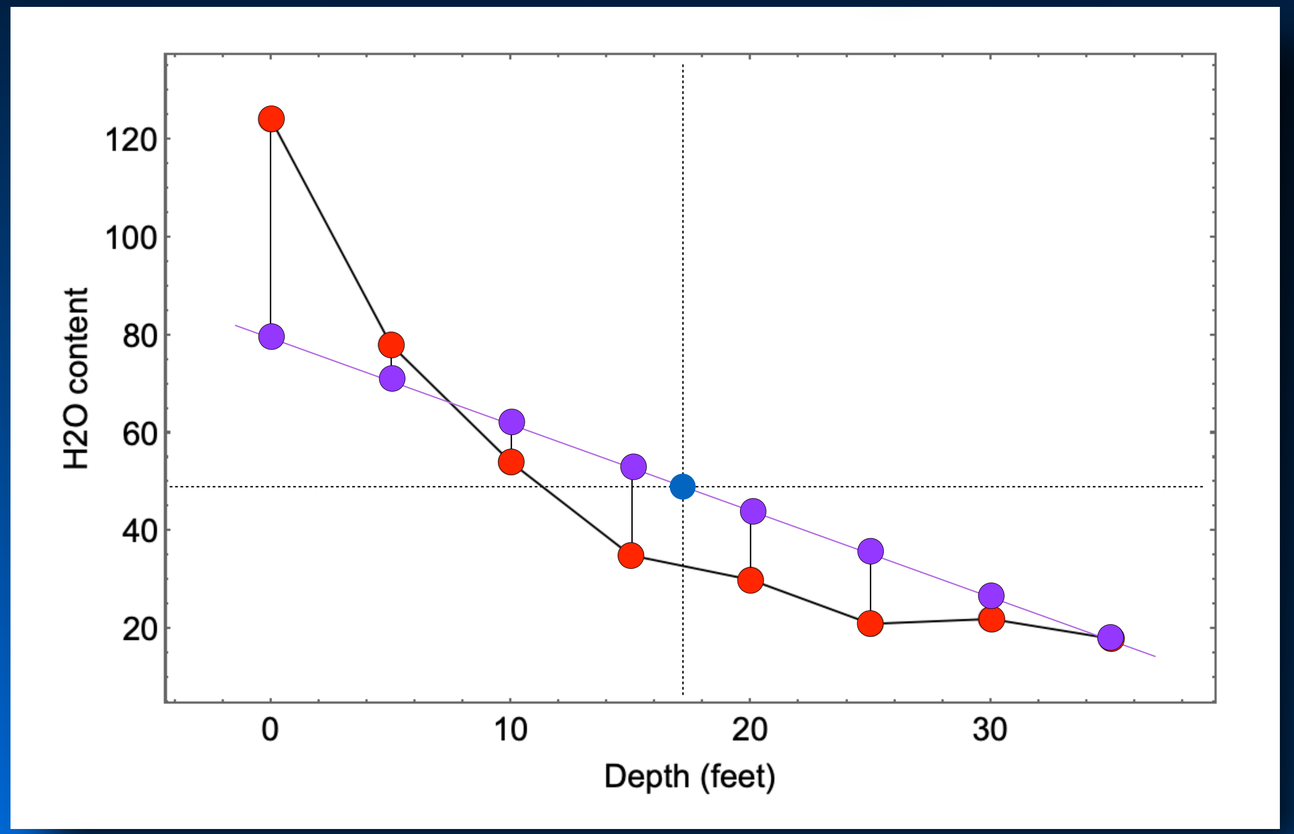

This orientation fits the data in the y direction better than the y on x model, but it doesn't fit the data in the x direction very well.

Linear Regression, Modeling & Testing

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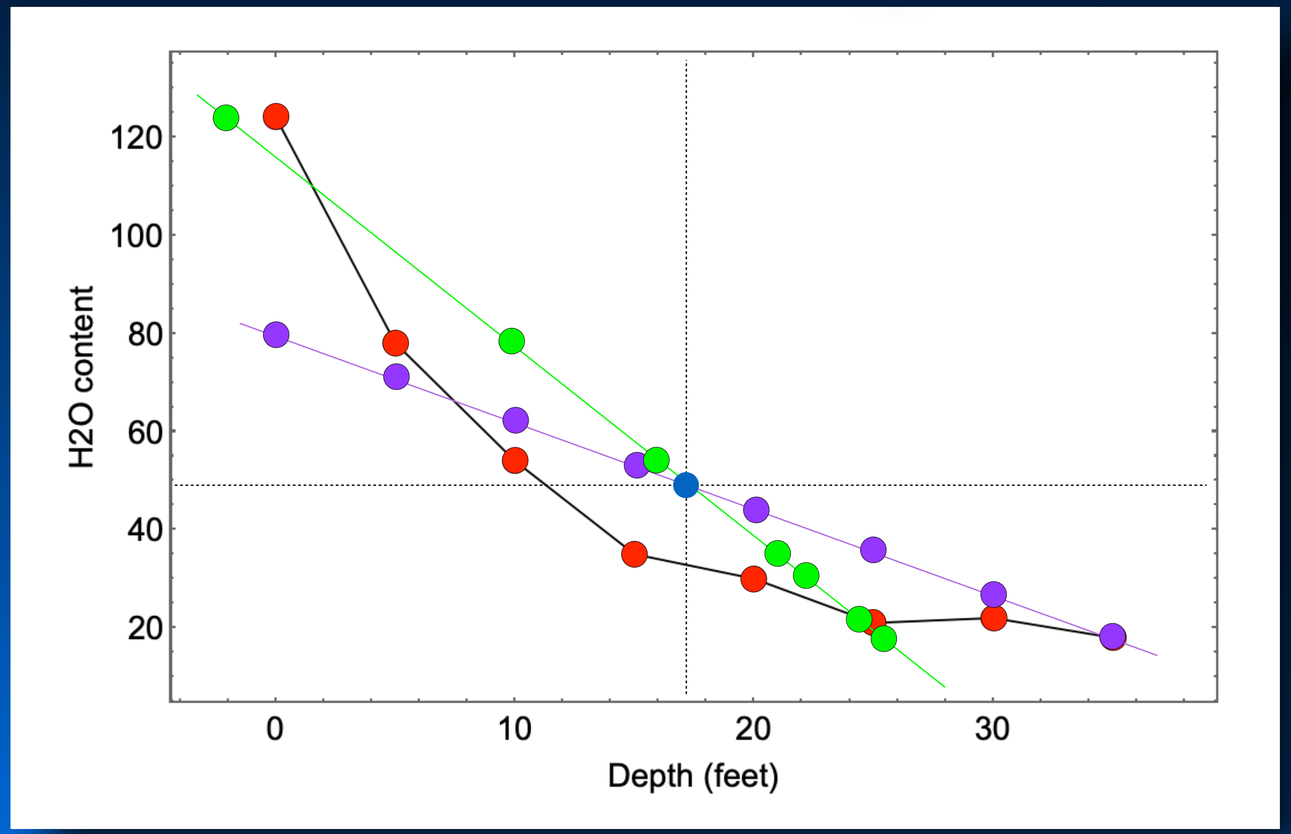

So, in order to choose between these two models we must decide which source of error we want to minimize.

Linear Regression, Modeling & Testing

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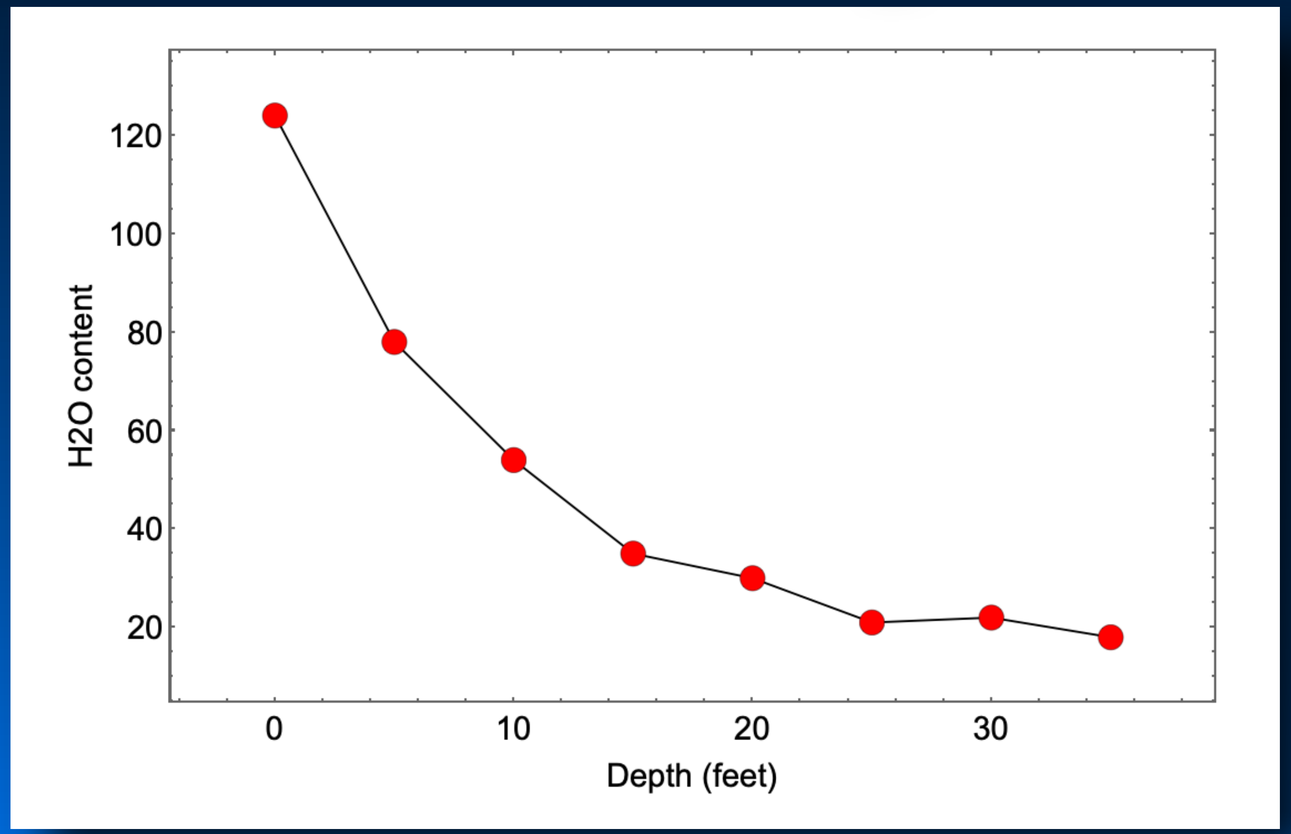

Independent variable = variable you know (not interested in its error).
Dependent variable = variable you wish to estimate (minimize its error).

Linear Regression, Modeling & Testing

Ordinary Least-Squares Linear Regression

i	Depth	H_20 Content	xy	$(x_{mean} - x)^2$
1	0	124	0	306.25
2	5	78	390	156.25
3	10	54	540	56.25
4	15	35	525	6.25
5	20	30	600	6.25
6	25	21	525	56.25
7	30	22	660	156.25
8	35	18	630	306.25
∑	140	382	3870	1050
∑/n	17.5	47.75		

$$y_i = \alpha + \beta x_i + \epsilon_i$$

Where: i = observation no.

α = y-intercept

β = slope

ϵ = error (residual)

$$\beta = \frac{\sum_{i=1}^{n} x_i y_i - ((\sum_{i=1}^{n} x_i \cdot \sum_{i=1}^{n} y_i)/n)}{\sum_{i=1}^{n} (\bar{x} - x_i)^2}$$

$$\alpha = \bar{y} - (\beta \cdot \bar{x})$$

When n = total number of observations

Linear Regression, Modeling & Testing

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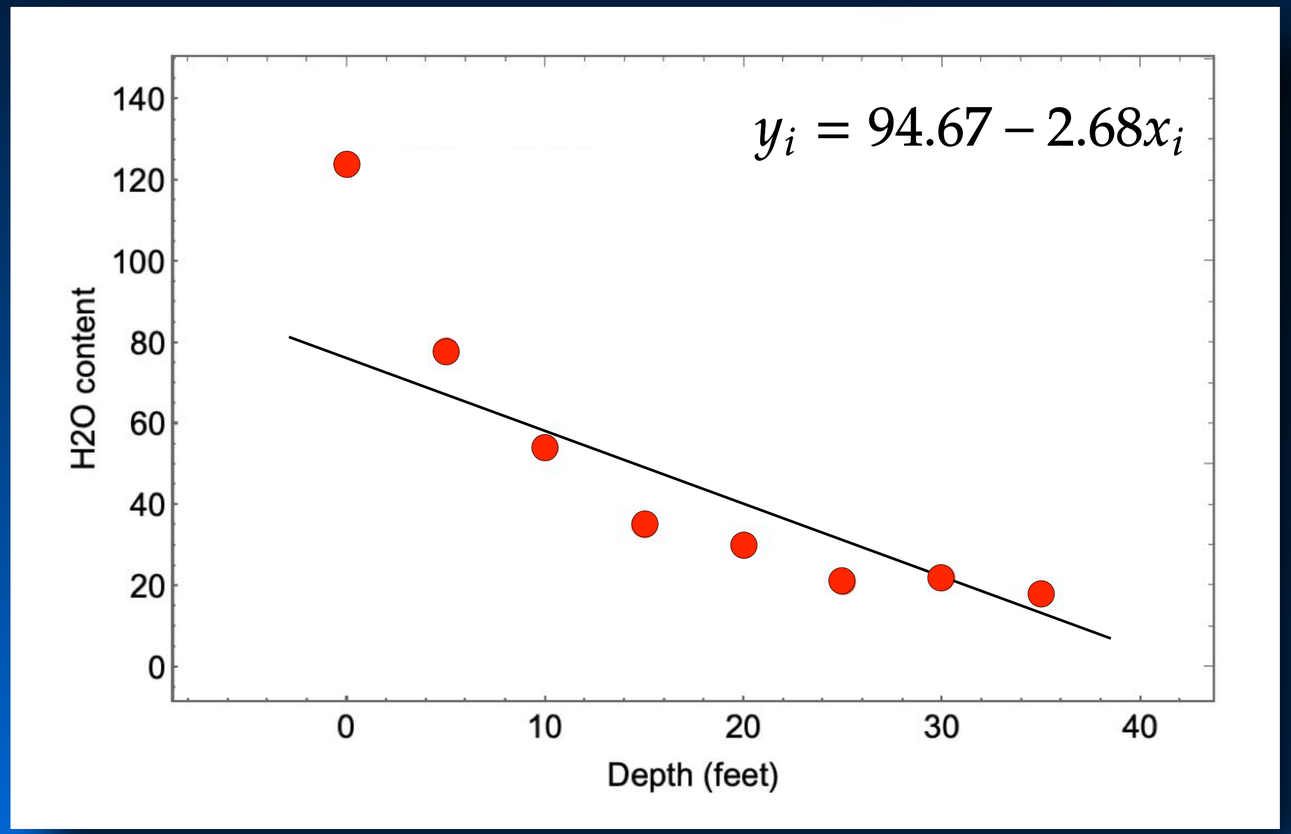

Independent variable = x variable. Dependent variable = y variable.

Linear Regression, Modeling & Testing

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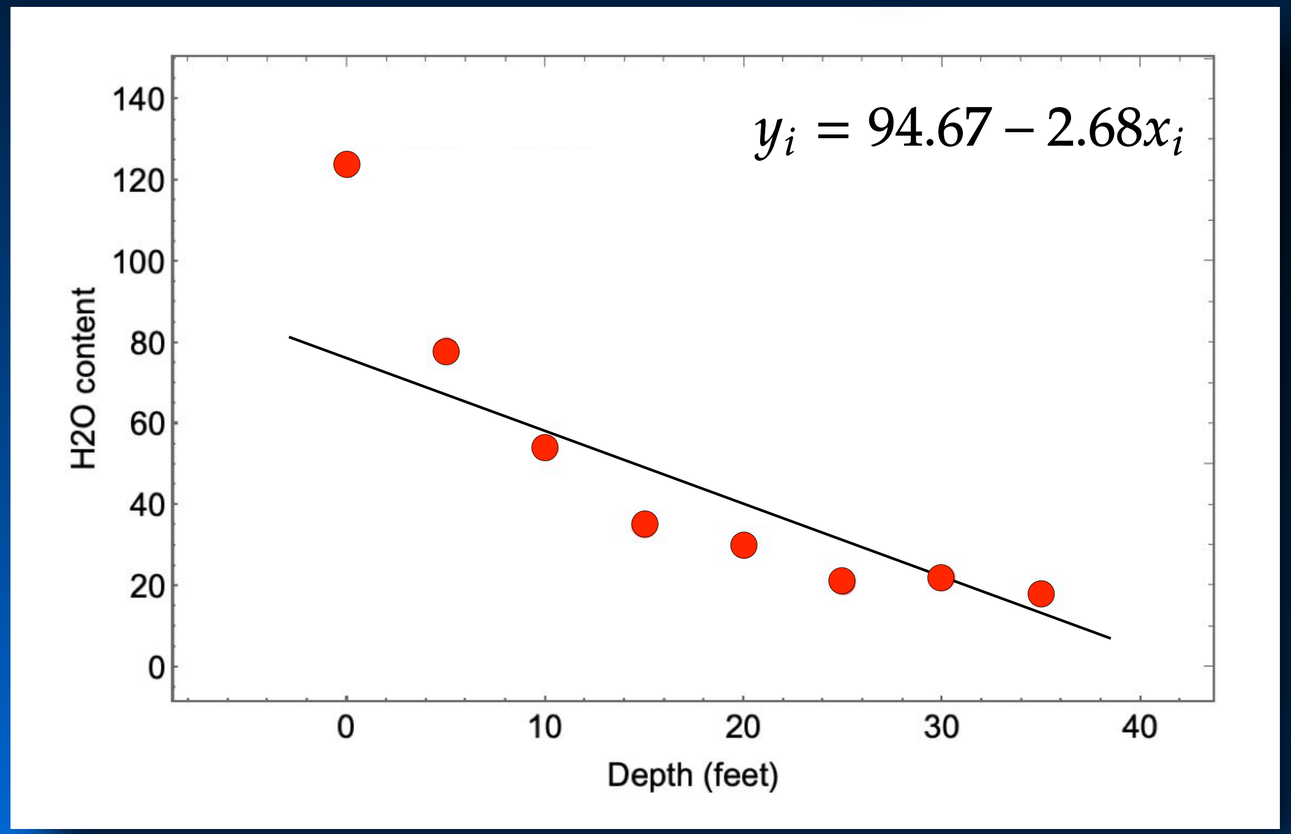


How well does this line (= linear model) fit these data? Is this fit significant statistically?

Linear Regression, Modeling & Testing

Analysis of Variance (ANOVA)

Developed originally by the English statistician Ronald A Fisher, ANOVA is based on the “law of total variance”. This holds the total variance of a dataset can be subdivided into components attributable to different sources. This is a very common principle that lies at the core of many statistical tests.

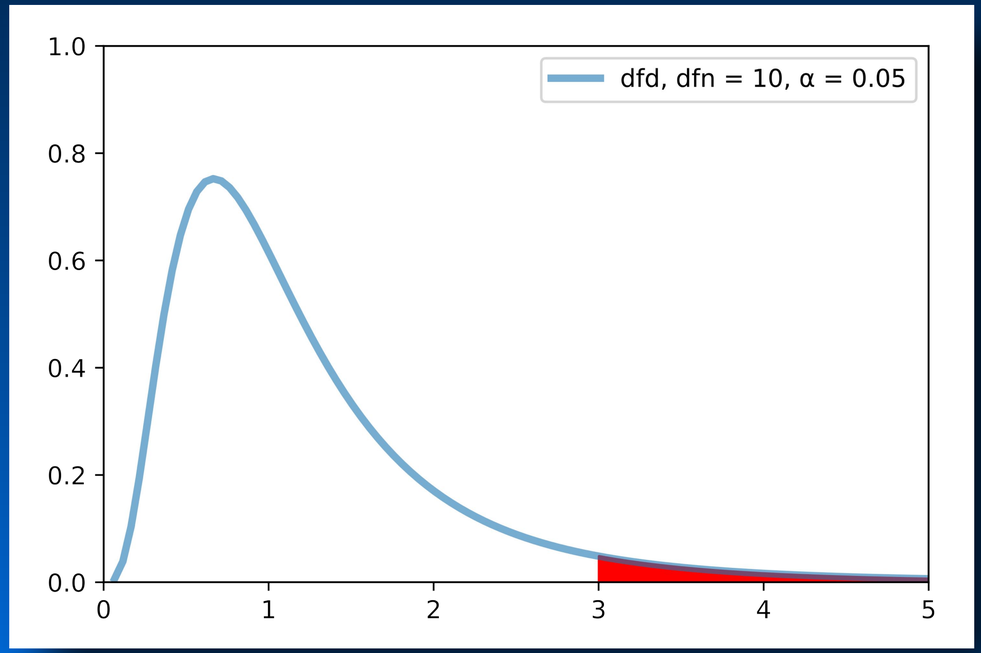
In the case of ANOVA determination of wether distinct components exist is made via compparison of the variance existing within data groups and the variance existing between data groups. So, unlike the t-Test, ANOVA tests the statements involving differences in the value of means by comparing variances.

R. A. Fisher
(1890-1962)

Linear Regression, Modeling & Testing

F-Test

In order to implement his ANOVA, Fisher developed the F-Test, which is based on a class of statistical distributions, the *F*-distribution.



R. A. Fisher
(1890-1962)

The F-distribution quantifies the probability of two independent variables having that same variances.

Linear Regression, Modeling & Testing

F-Test Assumptions

Like all statistical tests, Fisher's F-Test makes a variety of assumptions concerning the data. By performing an F-Test the statistician – or researcher – is implicitly claiming that their data conforms to these assumptions.

- Both datasets have been sampled from normally distributed populations.
- Samples have been selected independently from other samples.
- Variances of the populations being compared are equal.
- Samples have been selected randomly such that the overall sample forms a valid representation of the populations in question.

Linear Regression, Modeling & Testing

Analysis of Variance (ANOVA)

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	*F*-Test
Due to Model	SS_A	m-1	MS_A	MS_A/MS_E
Unexplained (Error)	SS_E	N-m	MS_E	
Total Variation	SS_T	N-1		

An ANOVA test is sometimes referred to as a “goodness of fit” test. It evaluates how much of the variance in a group or sample of observations can be represented by a particular explanation (or model) and how much is left unexplained (as “error”). The null hypotheses (H_0) is that there is no difference between these two variance values. Fisher’s F-test is used to evaluate this contention.

Linear Regression, Modeling & Testing

Analysis of Variance (ANOVA)

Source of Variation	Sum of Squares	Dof	Mean Squares	F Test
Due to Model	$SS_A = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$	$m - 1$	$MS_A = \frac{SS_A}{m-1}$	$\frac{MS_A}{MS_E}$
Unexplained (Error)	$SS_E = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2$	$N - m$	$MS_E = \frac{SS_E}{N-m}$	
Total Variation	$SS_T = \sum_{i=1}^{n} (y_i - \bar{y})^2$	$N - 1$		

Where: $\hat{y}$ = the estimated value of y;

$\bar{y}$ = the arithmetic mean of y;

m = number of variables;

n = number of samples.

Linear Regression, Modeling & Testing

Analysis of Variance (ANOVA)

Source of Variation	Sum of Squares	Dof	Mean Squares	F Test
Due to Model	7547.0	1	7547.0	23.072
Unexplained (Error)	1963.0	6	327.1	
Total Variation	9509.5	7		

$F_{0.05,\text{dof:}1,6} = 5.99$

$p_{F=23.072} = 0.003$

Very unlikely the estimated and residual variances are equal.

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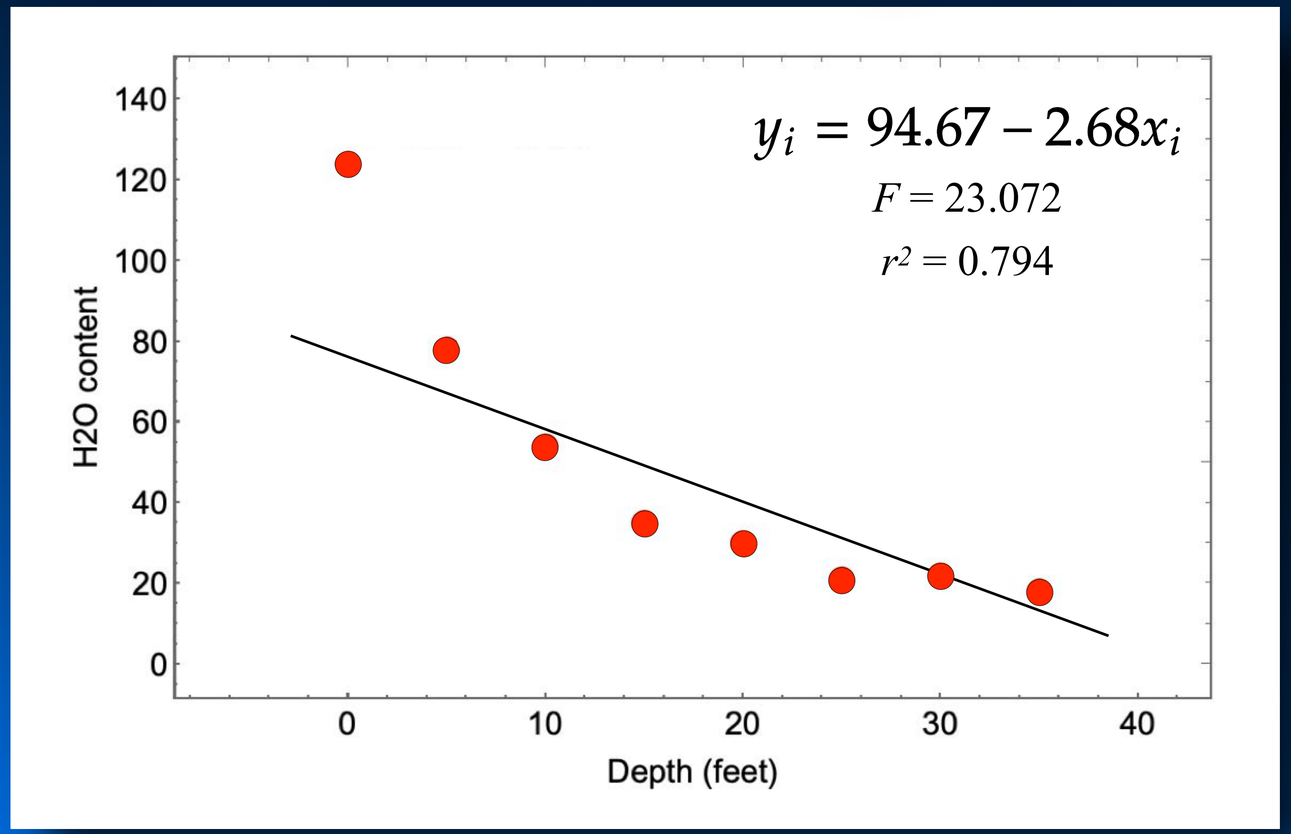


So, we are very confident a linear trend exists in these data and estimate we only have a 0.3% chance of being wrong … provided the assumptions we have made implicitly are correct.

Linear Regression, Modeling & Testing

Additional Linear Regression Statistics

Confidence Interval on the Slope - range of slopes within which the slope of the linear relationship of the population from which the sample was drawn lies.

Confidence Interval on the y-Intercept - range of y-intercepts within which the y-intercept of the linear relationship of the population from which the sample was drawn lies.

Coefficient of Dispersion - used to determine the degree to which data are clustered about the regression line; useful for comparing among different regression results.

Multiple Correlation Coefficient - a generalization of the standard or Pearson correlation coefficient; used to assess the quality of the prediction of the independent variable's (estimated) values.

Linear Regression, Modeling & Testing

Standard Error & Confidence Intervals

$$s_{\beta}^{2} = \frac{MS_E}{\sum_{i=1}^{n} x_i - \frac{(\sum_{i=1}^{n} x)^2}{n}}$$

$$b_{CI} = \pm\, t_{critialvalue} \cdot \sqrt{s_p^2}$$

$$\alpha_{CI} = \pm\, t_{critialvalue} \cdot \sqrt{MS_E \cdot \frac{\sum_{i=1}^{n} x^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2}}$$

Where: s_{β}^{2} = standard error of regression slope;

b_{CI} = confidence interval on regression slope;

α_{CI} = confidence interval on y-intercept.

Linear Regression, Modeling & Testing

Coefficients of Determination & Correlation

$$r^2 = \frac{SS_A}{SS_T}$$

$$r_{adj}^2 = \frac{SS_A}{SS_T} \cdot N\frac{(n-1)-1}{(N-1)-2}$$

$$r = \sqrt{r^2}$$

$$r_{adj} = \sqrt{r_{adj}^2}$$

Where: r^2 = coefficient of determination;

r_{adj}^2 = coefficient of determination (adjusted);

r = multiple correlation coefficient;

r_{adj} = multiple correlation coefficient (adjusted).

Linear Regression, Modeling & Testing

Depth vs H_20 Content of Louisiana Estuary Mud

Confidence Intervals (95%)

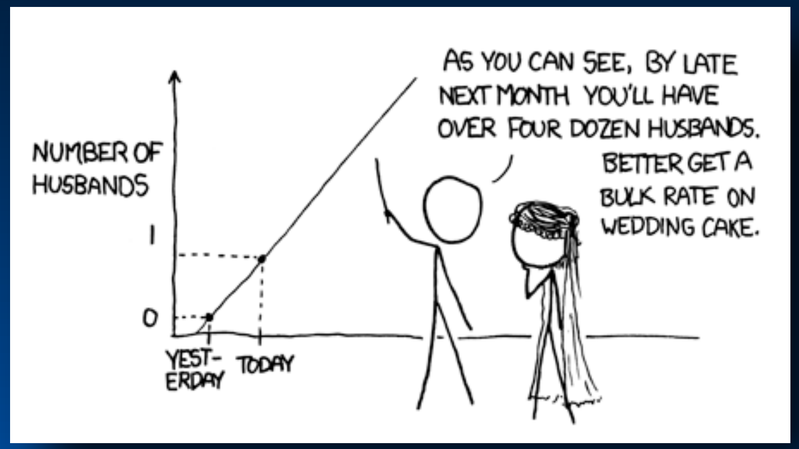
	y-Intercept (α)	Slope (β)
Upper	113.60	-3.77
Mean	94.67	-2.68
Lower	75.69	-1.60

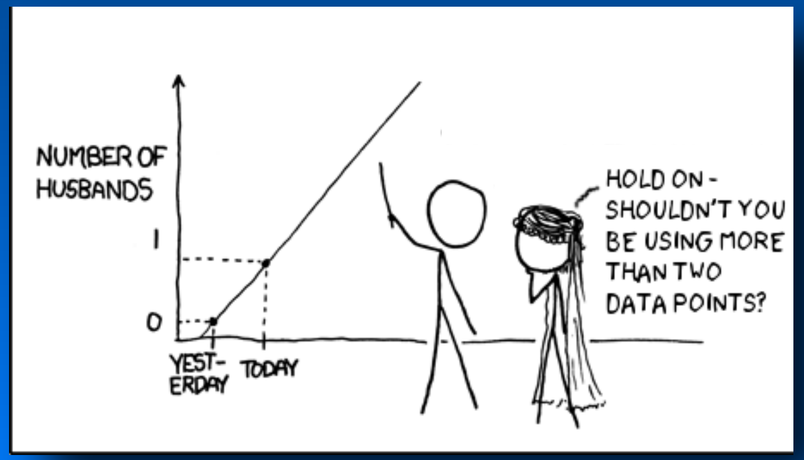
Measures of Dispersion

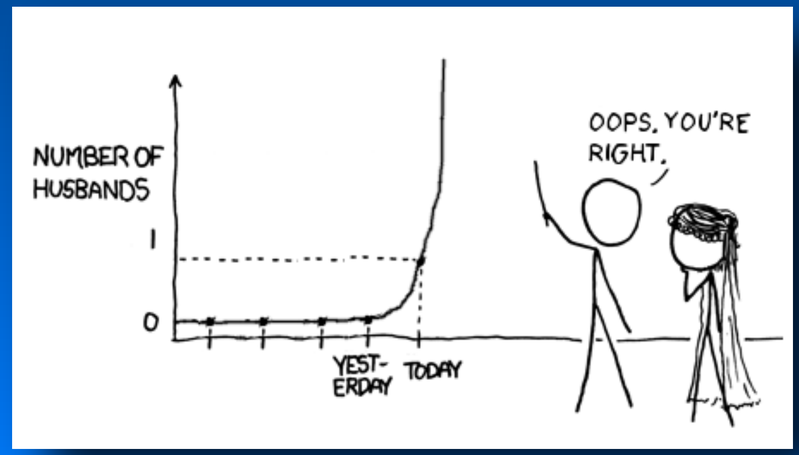
	Coefficient of Dispersion (r2)	Multiple Correlation Coefficient
Raw	0.794	0.891
Adjusted	0.926	0.962

Linear Regression, Modeling & Testing

So, is that all there is to know about linear regression analysis?







Linear Regression, Modeling & Testing

What about trilobites?

Genus	Length	Width
Acaste	5.10	3.46
Balizoma	4.60	6.53
Calymene	12.98	14.15
Ceraurus	7.90	5.32
Cheirurus	12.83	12.96
Cybantyx	16.41	13.08
Cybeloides	6.60	6.84
Dalmanites	10.00	9.12
Deiphon	8.08	10.77
Narroia	15.67	9.25
Ormathops	4.53	4.11
Phacopidina	6.44	6.94
Pricyclopyge	21.53	14.64
Ptychoparia	12.82	9.36
Rhenops	22.27	17.56
Sphaerexochus	4.93	6.21
Trimerus	16.35	15.02
Zachanthoides	13.41	8.51

Flexicalymene

Linear Regression, Modeling & Testing

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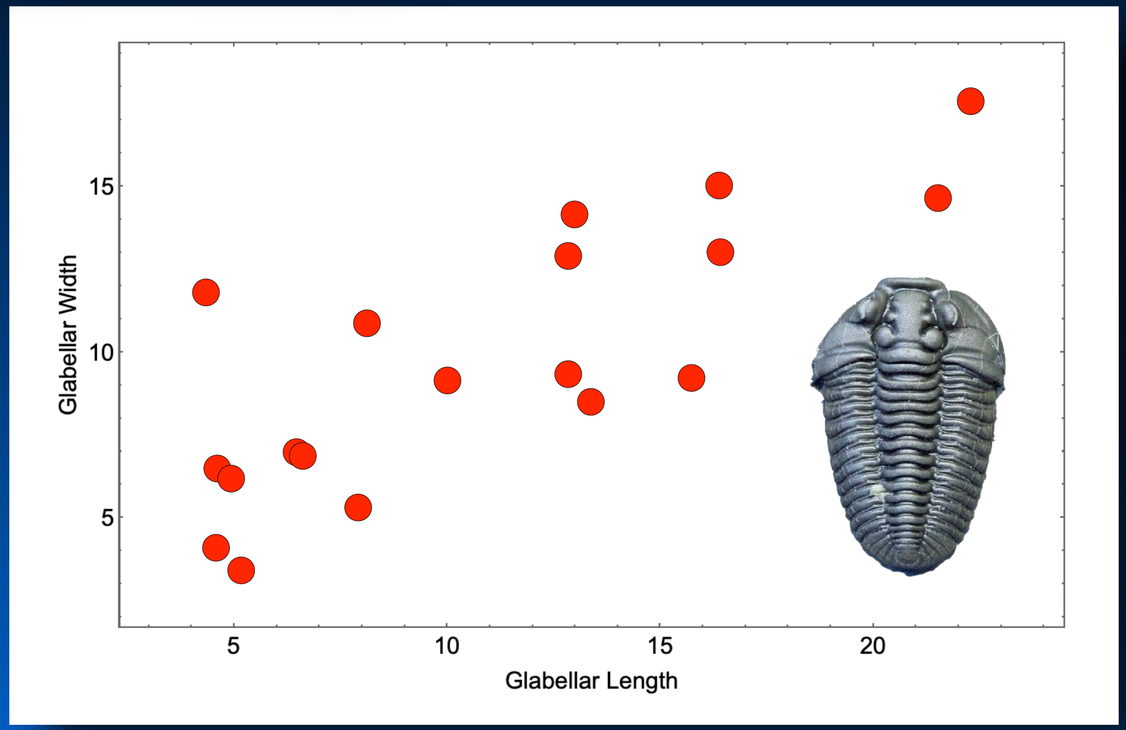
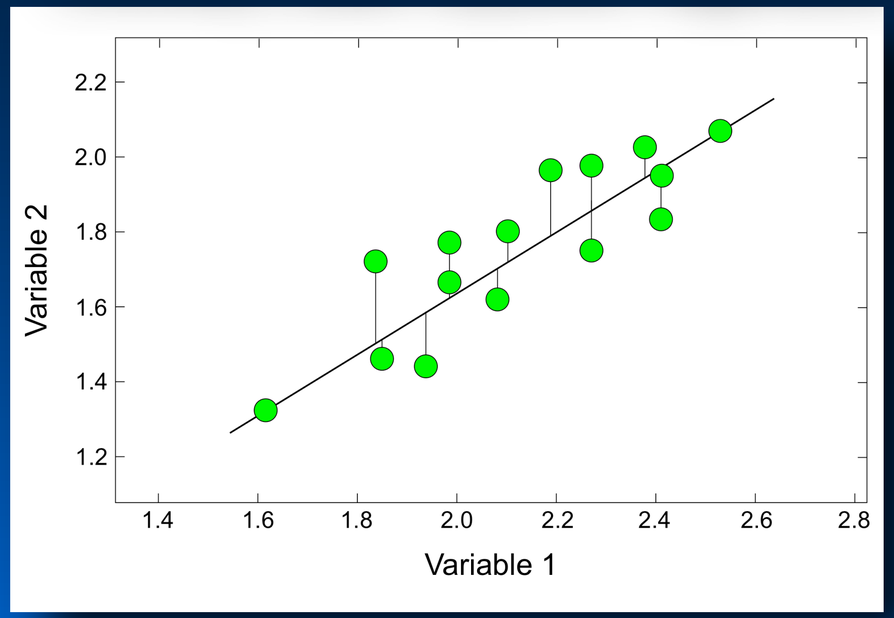


Which one's the independent variable?
Glabellar length?
Glabellar width?

Linear Regression, Modeling & Testing

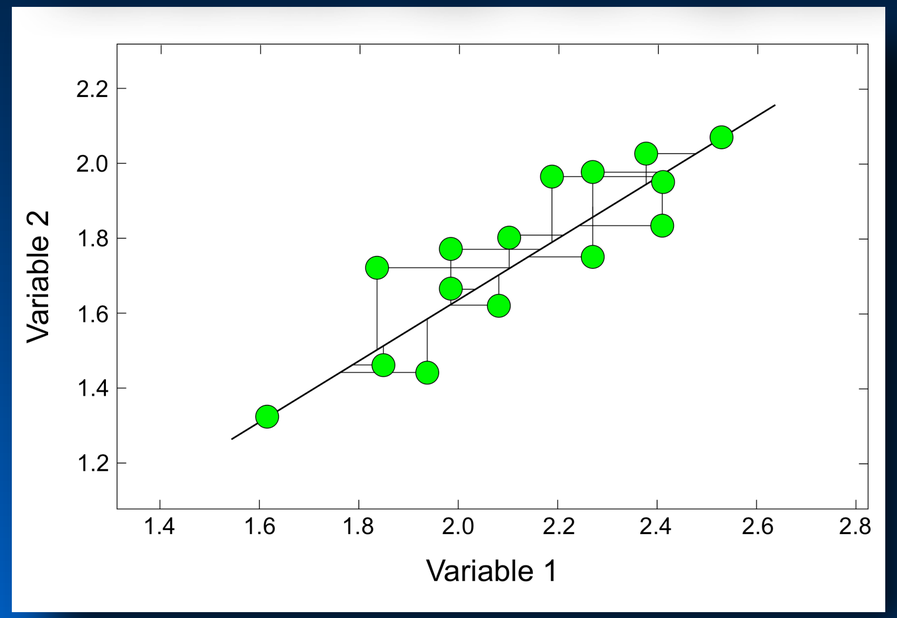
Alternative Regression Error Minimization Strategies

Ordinary Least Squares Regression



Also called:
Regression
Least Squares Regression
Model I Regression

Standardized Major Axis Regression



Also called:
Reduced Major Axis Regression
Geometric Mean Regression
Model II Regression

Linear Regression, Modeling & Testing

Standardized Major Axis Linear Regression

Genus	Length	Width	Dev_L	Dev_W	SDP
Acaste	5.10	3.46	-6.15	-6.20	38.10
Balizoma	4.60	6.53	-6.65	-3.13	20.79
Calymene	12.98	14.15	1.73	4.49	7.78
Ceraurus	7.90	5.32	-3.35	-4.34	14.52
Cheirurus	12.83	12.96	1.58	3.30	5.23
Cybantyx	16.41	13.08	5.16	3.42	17.67
Cybeloides	6.60	6.84	-4.65	-2.82	13.09
Dalmanites	10.00	9.12	-1.25	-0.54	0.67
Deiphon	8.08	10.77	-3.17	1.11	-3.52
Narroia	15.67	9.25	4.42	-0.41	-1.80
Ormathops	4.53	4.11	-6.72	-5.55	37.26
Phacopidina	6.44	6.94	-4.81	-2.72	13.06
Pricyclopyge	21.53	14.64	10.28	4.98	51.24
Ptychoparia	12.82	9.36	1.57	-0.30	-0.47
Rhenops	22.27	17.56	11.02	7.90	87.11
Sphaerexochus	4.93	6.21	-6.32	-3.45	21.78
Trimerus	16.35	15.02	5.10	5.36	27.37
Zachanthoides	13.41	8.51	2.16	-1.15	-2.48
Sum	202.45	173.83	0.00	0.00	
Mean	11.25	9.66	0.00	0.00	
Std. Dev.	5.67	4.11	5.67	4.11	

$$\beta = \frac{4.11}{5.67}$$

$$\alpha = \bar{y} - (\beta \cdot \bar{x})$$

When n = total number of observations

$$SDP = \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})$$

Sign of slope (β) = sign of SDP

Linear Regression, Modeling & Testing

Standardized Major Axis Linear Regression

$$\beta = \frac{s_y}{s_x}$$

$$\beta = \frac{s_y}{s_x} = 0.72$$

$$\alpha = \bar{y} - (\beta \cdot \bar{x})$$

When n = total number of observations

$$\alpha = 9.66 - (0.72 \cdot 11.25)$$

$$a = 1.51$$

$$SDP = \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})$$

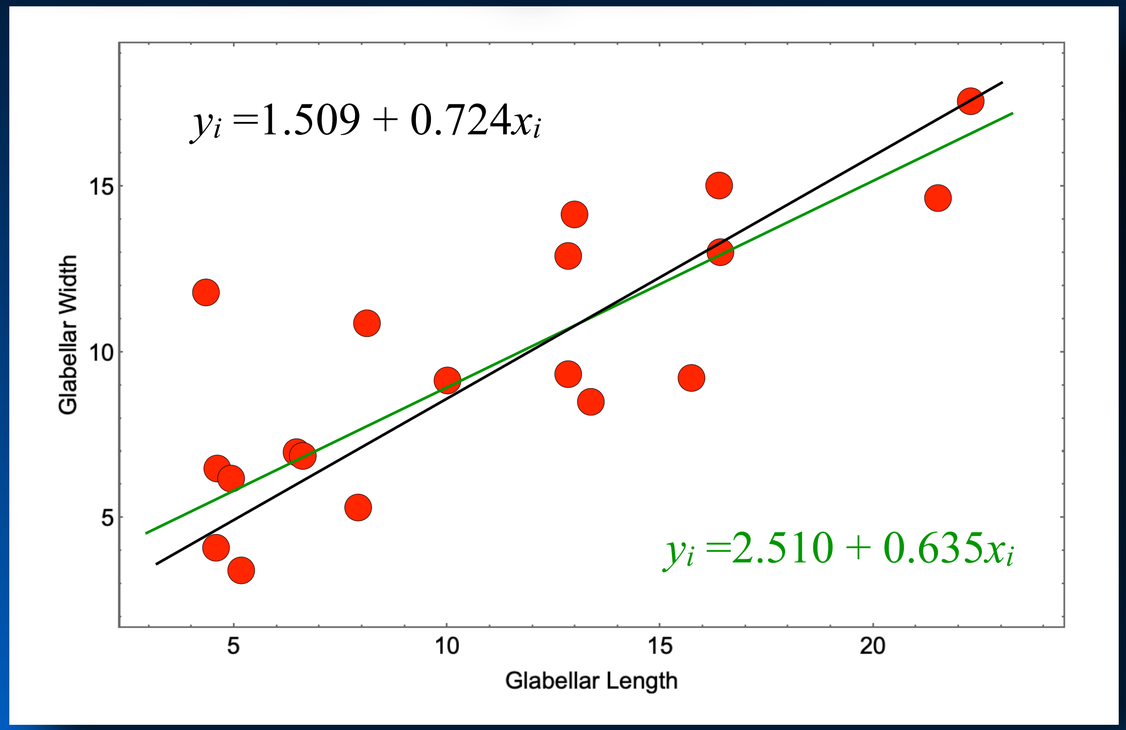
$$SDP = 347.39$$

Sign of slope (β) = sign of SDP

Linear Regression, Modeling & Testing

Standardized Major Axis Linear Regression

Genus	Length	Width
Acaste	5.10	3.46
Balizoma	4.60	6.53
Calymene	12.98	14.15
Ceraurus	7.90	5.32
Cheirurus	12.83	12.96
Cybantyx	16.41	13.08
Cybeloides	6.60	6.84
Dalmanites	10.00	9.12
Deiphon	8.08	10.77
Narroia	15.67	9.25
Ormathops	4.53	4.11
Phacopidina	6.44	6.94
Pricyclopyge	21.53	14.64
Ptychoparia	12.82	9.36
Rhenops	22.27	17.56
Sphaerexochus	4.93	6.21
Trimerus	16.35	15.02
Zachanthoides	13.41	8.51



Note: the standardized major axis regression line is usually closer to the line we'd draw by eye than the least-squares regression line.

Linear Regression, Modeling & Testing

Standardized Major Axis Linear Regression

Source of Variation	Sum of Squares	DoF	Mean Squares	F Test
Due to Model	$SS_A = \sum_{i=1}^{n} ((\hat{x}_i, \hat{y}_i) - (\bar{x}_i, \bar{y}_i))^2$	$m-1$	$MS_A = \frac{SS_A}{m-1}$	$\frac{MS_A}{MS_E}$
Unexplained (Error)	$SS_A = \sum_{i=1}^{n} ((x_i, y_i) - (\hat{x}_i, \hat{y}_i))^2$	$N-m$	$MS_E = \frac{SS_E}{N-m}$	
Total Variation	$SS_T = \sum_{i=1}^{n} ((x_i, y_i) - (\bar{x}_i, \bar{y}_i))^2$	$N-1$		

Linear Regression, Modeling & Testing

Standardized Major Axis Linear Regression

Source of Variation	Sum of Squares	DoF	Mean Squares	F Test
Due to Model	269.3	1	269.3	244.5
Unexplained (Error)	17.6	16	1.01	
Total Variation	286.9	17		

$F_{0.05,\text{dof:}1,6} = 4.49$

$p_{F=244.5} = 0.0000$

Very, very unlikely the estimated and residual variances are equal.

Linear Regression, Modeling & Testing

Standardized Major Axis Linear Regression

Confidence Intervals (95%)

	y-Intercept (α)	Slope (β)
Upper	3.323	0.93
Mean	1.51	0.72
Lower	-0.825	0.56

Measures of Dispersion

	Coefficient of Dispersion (r^2)	Multiple Correlation Coefficient
Raw	0.939	0.969
Adjusted	0.997	0.999

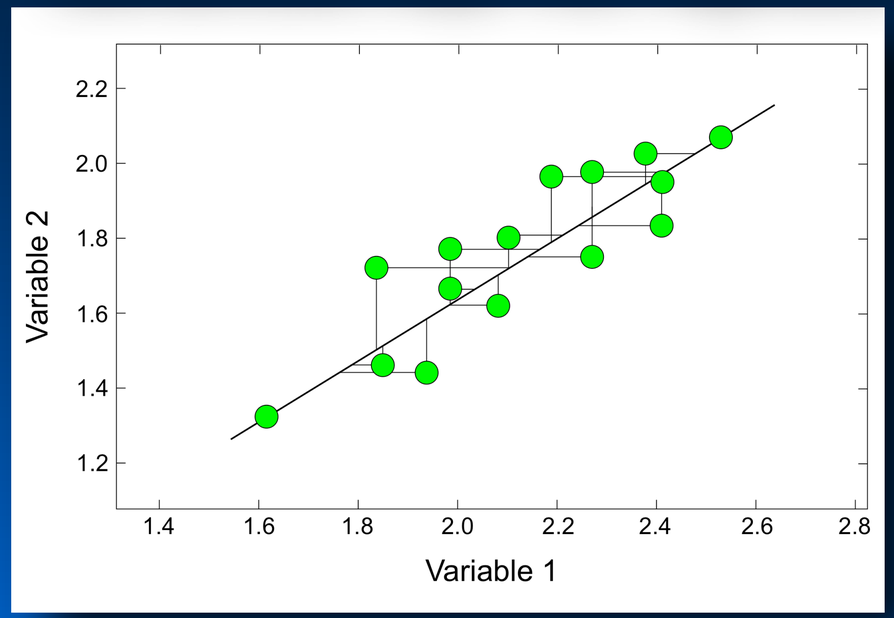
Linear Regression, Modeling & Testing

SMA regression is too simple. Don’t you have anything more complex?

Linear Regression, Modeling & Testing

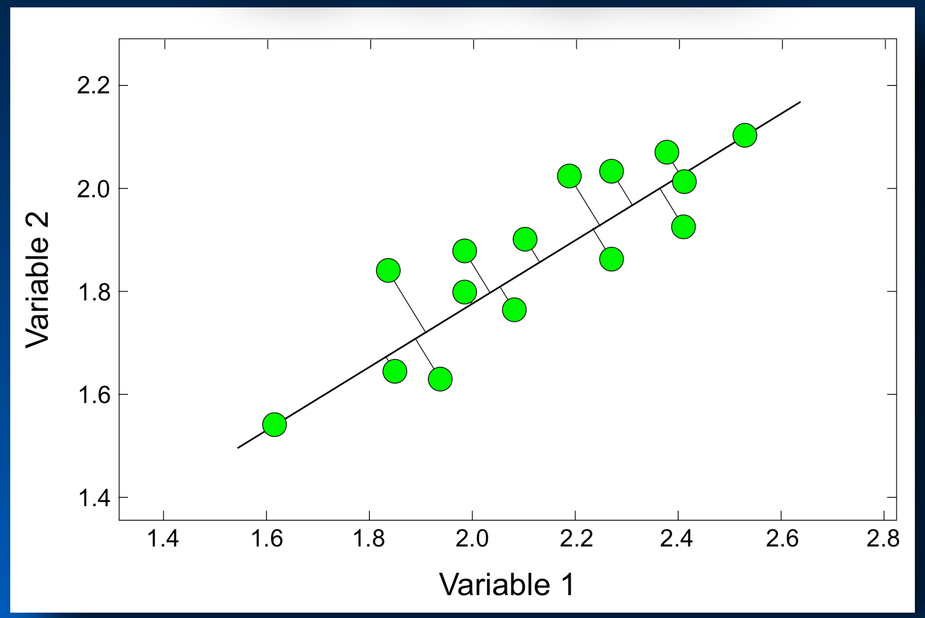
Additional Regression Error Minimization Strategies

Standardized Major Axis Regression



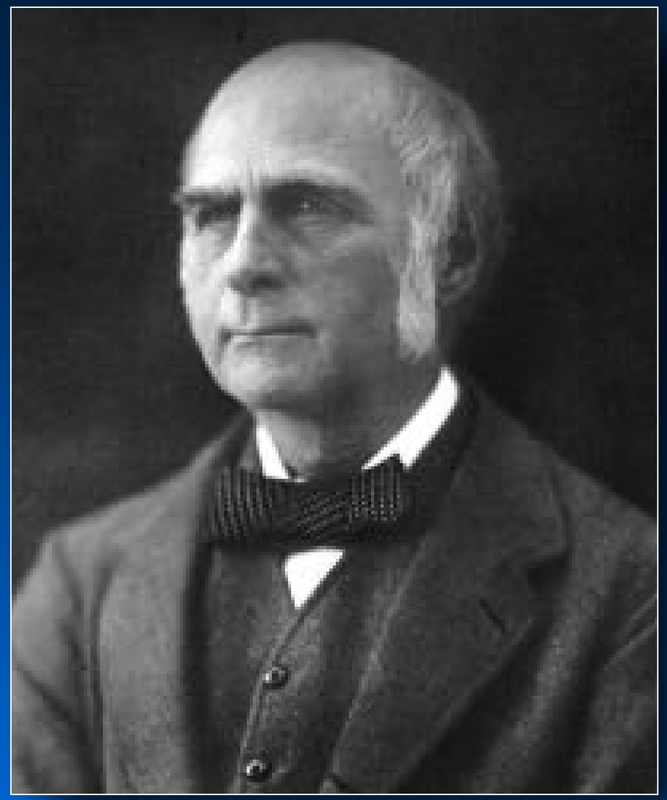
Also called:
Reduced Major Axis Regression
Geometric Mean Regression
Model II Regression

Major Axis Regression



Also called:
Structural Analysis, Orthogonal Regression, Bivariate PCA
Model II Regression

Bivariate Regression, Modeling & Testing of Earth Science Data



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