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January 11, 2021

Biol 520C: Statistical modelling for biological data

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- You also have digital access to the textbooks I mentioned for free through the UBCO Library:

https://muse-jhu-edu.ezproxy.library.ubc.ca/book/33194

https://link-springer-com.ezproxy.library.ubc.ca/book/10.1007%2F978-0-387-87458-6

https://www-degruyter-com.ezproxy.library.ubc.ca/princetonup/view/title/563354





 Practical 01 is up on the course website, and will be unlocked on Canvas after today's lecture. It is due before the start of the lecture next Tuesday.

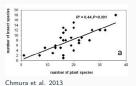


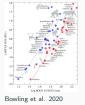


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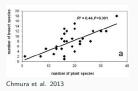


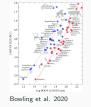


Johnson et al. 2017



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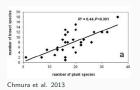


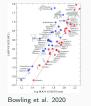


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Our verbal hypothesis in this case is 'X is proportional to Y'. But looking at the data isn't enough. So how do we approach the problem statistically?





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The method itself isn't simple and there's a lot going on under the hood.





Data is of the form:

$$d = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}\$$

$$\begin{array}{ccc}
X & Y \\
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Verbal description of the hypothesis:

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Regression Model



More formally, a straight line is described by an intercept (β_0) and a slope (β_1) : $y_i = \beta_0 + \beta_1 x_i$

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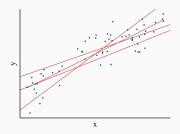
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With data $d = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, the question is what values of β_0 and β_1 best describe the relationship between x and y (i.e., what line do you draw through the data?)







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Source: www.constellation-guide.com



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In 1805, Legendre published an algebraic procedure for fitting linear equations to data. His 'least squares' approach assumed each observation y_i is accompanied by some amount of noise ε_i . If you further constrain the problem such that the sum of the squared errors needs to be minimized, only one line fits the data.



Source: www.constellation-guide.com



Source: Wikipedia

Least Squares Fitting Cont.

For a given observation, a line predicts y_i to be $\beta_0 + x_i \beta_1$.

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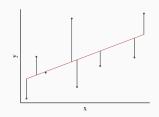


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We want to find the value for β_0 and β_1 that minimizes this quantity.



Parameter estimation



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One solution is to calculate $\sum_{i=1}^{n} (y_i - (\beta_0 + x_i\beta_1))^2$ for all values of β_0 and β_1 between $-\infty$ and ∞ .

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But who wants to do that?

Matrix Algebra Review





Matrices are rectangular collections of numbers, generally denoted via bold capital letters.

$$A = \begin{pmatrix} 2 & 7 & -3 & 4 \\ -7 & 1 & 1 & 8 \\ -9 & 4 & 5 & -1 \end{pmatrix}$$

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So here, $a_{3,2} = 4$, and $a_{1,3} = -3$.

Vectors



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'Ordinary' numbers can be thought of as a 1×1 matrices, or scalars (e.g., D=7).





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$$A + B = \begin{pmatrix} 1 & -5 & 4 \\ 2 & 5 & 3 \end{pmatrix} + \begin{pmatrix} 8 & -3 & -4 \\ 4 & -2 & 9 \end{pmatrix}$$



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Matrix addition has many of the same properties as normal addition.

$$A + B = B + A$$
$$A + (B + C) = (A + B) + C$$





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If a matrix is its own transpose, then that matrix is said to be symmetric, e.g.:

$$A = \begin{pmatrix} 1 & -5 & 4 \\ -5 & 7 & 3 \\ 4 & 3 & 3 \end{pmatrix} = A' = A^T$$







$$6 \times A = 6 \times \begin{pmatrix} 1 & -5 & 4 \\ 2 & 5 & 3 \end{pmatrix}$$



$$6 \times A = 6 \times \begin{pmatrix} 1 & -5 & 4 \\ 2 & 5 & 3 \end{pmatrix} = \begin{pmatrix} 6 \times 1 & 6 \times -5 & 6 \times 4 \\ 6 \times 2 & 6 \times 5 & 6 \times 3 \end{pmatrix}$$



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To multiply a matrix by a scalar, also known as scalar multiplication, multiply every element in the matrix by the scalar.

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To perform matrix multiplication, the first matrix must have the same number of columns as the second matrix has rows. The dimensions of the resulting matrix equals the number of rows of the first matrix, and the number of columns of the second matrix (e.g., a 3×5 matrix \times a 5×7 matrix = a 3×7 matrix).





$$C \times D = \begin{pmatrix} 3 & -9 & -8 \\ 2 & 4 & 3 \end{pmatrix} \times \begin{pmatrix} 7 & -3 \\ -2 & 3 \\ 6 & 2 \end{pmatrix}$$



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$$\begin{pmatrix} 21+18-48 & -9-27-16 \\ 14-8+18 & -6+12+6 \end{pmatrix} = \begin{pmatrix} -9 & -52 \\ 24 & 12 \end{pmatrix}$$

Matrix Properties



Matrix Properties



An identity matrix is a square matrix where every diagonal entry is 1 and all the other entries are 0

$$I = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

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The trace of a $n \times n$ matrix is the sum of all the diagonal entries. In other words, for $n \times n$ matrix $trace(A) = tr(A) = \sum_{i=1}^{n} a_{i,i}$

$$tr(I) = tr \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1 + 1 + 1 = 3$$





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Inverting matrices requires a complicated algorithm, so we usually rely on computers to perform the calculations (e.g. the solve() function in R).

Linear regression and matrix

notation





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The observations of the response variable y are grouped into a single column, $n \times 1$, matrix

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The regression coefficients β_0 and β_1 are grouped into a 2×1 matrix

$$\beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$



Given our dataset $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ we can re-write x, y, and our regression parameters as matrices:

The observations of the response variable y are grouped into a single column, $n \times 1$, matrix

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

The regression coefficients β_0 and β_1 are grouped into a 2×1 matrix

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The observations of the predictor are grouped into a two column, $n \times 2$ matrix.

$$\mathbf{x} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$$



Why the column of 1s in x?



Why the column of 1s in x? When we multiply x by β we get:

 $x\beta$



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$$\times \beta = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \times \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} 1 \times \beta_0 + x_1 \times \beta_1 \\ 1 \times \beta_0 + x_2 \times \beta_1 \\ \vdots \\ 1 \times \beta_0 + x_n \times \beta_1 \end{pmatrix} = \begin{pmatrix} \beta_0 + \beta_1 x_1 \\ \beta_0 + \beta_1 x_2 \\ \vdots \\ \beta_0 + \beta_1 x_n \end{pmatrix}$$





At each data point, our model results in some amount of error in the prediction, so we have n errors. These form a vector:

$$\varepsilon = \mathbf{y} - \mathbf{x}\boldsymbol{\beta}$$



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So our original regression problem in matrix notation is:

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$





So how does this help us estimate our regression parameters?

Linear regression in matrix notation



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We can also rewrite our sum of squares equation in matrix form

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So instead of plugging in all of the possible values of β_0 and β_1 between $-\infty$ and ∞ to obtain our parameter estimates, all we have to do is a matrix calculation.

Assumptions of linear regression





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Just because a specific estimator makes assumptions that aren't met by real data, this doesn't mean that the relationship doesn't exists or that the estimator is useless, but it does tell you that your estimator can be improved.





Applying linear regression to a problem relies on satisfying 5 assumptions:

• Correct model specification



- Correct model specification
- Normality of the residuals



- Correct model specification
- Normality of the residuals
- Homogeneity



- Correct model specification
- Normality of the residuals
- Homogeneity
- Fixed x



- Correct model specification
- Normality of the residuals
- Homogeneity
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- Independence





In model based inference we need to apply some sort of model to our data.



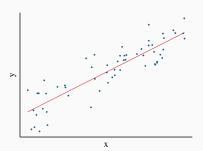
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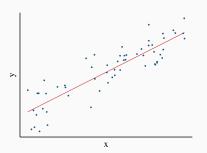
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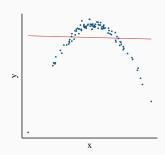




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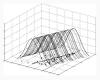
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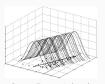


Source: Zuur et al. (2009)



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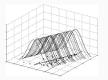
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In practice, we usually don't have many repeat measures of a specific \boldsymbol{x} value, so checking for this usually means pooling all of the residuals and checking for normality. Normality of pooled residuals is reassuring, but does not necessarily mean the population is normally distributed.





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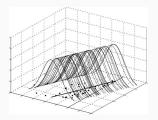


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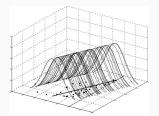


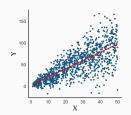
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What will heterogeneity do to your estimates?

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If you have defined the exact values at which x and y are measured, and there is no measurement error, this assumption is perfectly fine.

Situations where x is accompanied by a meaningful amount measurement error can break this assumption.





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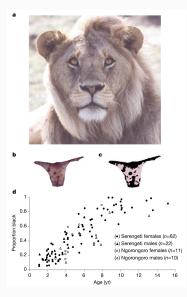
The standard deviation is given by: $\sigma = \sqrt{\frac{\sum (x_i - \mu)^2}{n}}$, what effect does breaking the assumption of independence have?

Linear regression example

Example: Lion noses



The Problem: In lion populations, the sustainable application of trophy hunting is often used as a way of maintaining stable populations while generating valuable funds to support conservation efforts. If you hunt older lions that are past their reproductive prime, the impact on the population is negligible, but if you hunt lions that are too young, there is a risk of the population destabilising. Whitman et al. (2004) looked at whether there was a relationship between how black a male lion's nose was and its age.



Lion noses: the data



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	proportionBlack	Age
ſ	0.21	1.1
	0.14	1.5
	0.11	1.9
	0.13	2.2
	0.12	2.6
	0.13	3.2
	0.12	3.2
	0.18	2.9
	0.23	2.4
	0.22	2.1
	0.2	1.9
	0.17	1.9
	0.15	1.9
	0.27	1.9
	0.26	2.8
	0.21	3.6
	0.3	4.3
	0.42	3.8
	0.43	4.2
	0.59	5.4
	0.6	5.8
	0.72	6
	0.29	3.4
	0.1	4
	0.48	7.3
	0.44	7.3
	0.34	7.8
	0.37	7.1
	0.34	7.1
	0.74	13.1
	0.79	8.8
	0.51	5.4

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0.51	5.4

The regression problem in matrix notation is:

$$\begin{pmatrix} 0.21 \\ 0.14 \\ \vdots \\ 0.51 \end{pmatrix} = \begin{pmatrix} 1 & 1.1 \\ 1 & 1.5 \\ \vdots & \vdots \\ 1 & 5.4 \end{pmatrix} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

Lion noses: Estimating the parameters



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which gives us $\beta_0 = 0.06969626$ and $\beta_1 = 0.05859115$

Lion noses: Estimating the parameters



Lion noses: Estimating the parameters



We can also do this the easy way by using the lm() function:

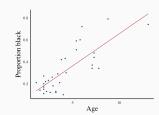
```
lm(proportionBlack ~ ageInYears, data = data)
```



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```
Call.
lm(formula = proportionBlack ~ ageInYears, data = data)
Residuals:
     Min
                    Median
                                         Max
               10
-0.20406 -0.07758 -0.01750 0.07913 0.29876
Coefficients:
            Estimate Std. Error t value Pr(>t)
(Intercept) 0.069696
                       0.041956
                                  1.661
                                           0.107
ageInYears 0.058591
                       0.008307
                                  7.053 7.68e-08 ***
Signif. codes: 0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1
Residual standard error: 0.1238 on 30 degrees of freedom
Multiple R-squared: 0.6238, Adjusted R-squared: 0.6113
F-statistic: 49.75 on 1 and 30 DF, p-value: 7.677e-08
```

lm(proportionBlack ~ ageInYears, data = data)





The least squares method provides a path for parametrising a model's deterministic component



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To solve this issue, we need to approach the problem as probalists and assume that each error term ε_i comes from some distribution ϕ .



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We'll continue along this train of thought next lecture.