Multiple Linear Regression

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Biol 520C: Statistical modelling for biological data

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Housekeeping

- Datasets for papers: consider asking your supervisor or lab mates for data on your study system.

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For some systems knowing the relationship between X and Y is sufficient, but in most biological systems there are typically multiple variables that influence outcomes (e.g., rainfall, sunlight, soil composition all influence plant growth)

Our verbal hypothesis in this case is 'Y is proportional to X_1, X_2, ... X_m'. With multiple factors, how do we approach the problem statistically?

Remembering that for simple linear regression our data is of the form:

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

X	Y
x_1	y_1
x_2	y_2
$\ldots$	$\ldots$
x_n	y_n

And our relationship is described by an intercept (β_0) and a slope (β_1):

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

For m explanatory variables, the data are of the form:

Y	X_1	X_2	...	X_m
y_1	X_{11}	X_{21}	...	X_m1
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A linear regression with multiple explanatory variables is described by an intercept (β_0) and a regression coefficients ($\beta_1, \beta_2, \ldots, \beta_m$):

$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_m x_{mi} + \varepsilon_i$

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x = \begin{pmatrix} 1 & x_1 1 & x_2 1 \\ 1 & x_1 2 & x_2 2 \\ \vdots & \vdots & \vdots \\ 1 & x_1 n & x_2 n \end{pmatrix}
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$$

Notice how the dimensions of the matrices all line up, so even though we've added new parameters we can still estimate their values using our old friend $\beta = (x^Tx)^{-1}x^Ty$.

Multiple Linear Regression

Pre-analysis

With only one parameter, there is only a single relationship that is possible

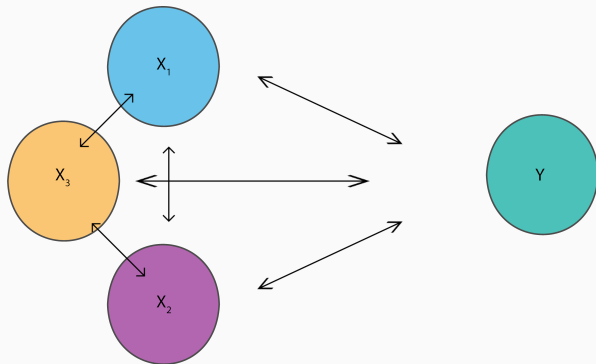With only one parameter, there is only a single relationship that is possible
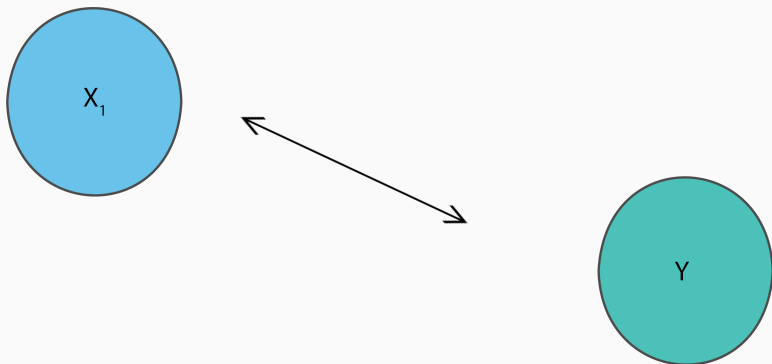
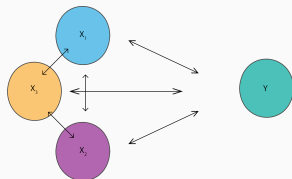With two parameters, there are 3 relationship that are possible
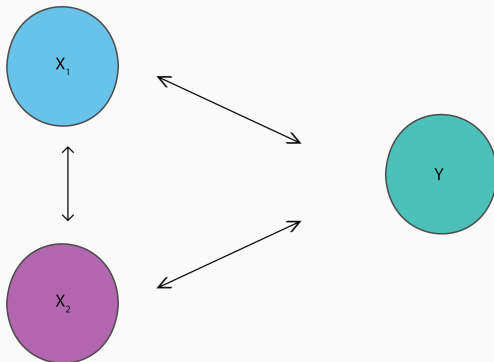
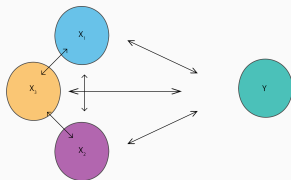With three parameters, there are 6 relationship that are possible
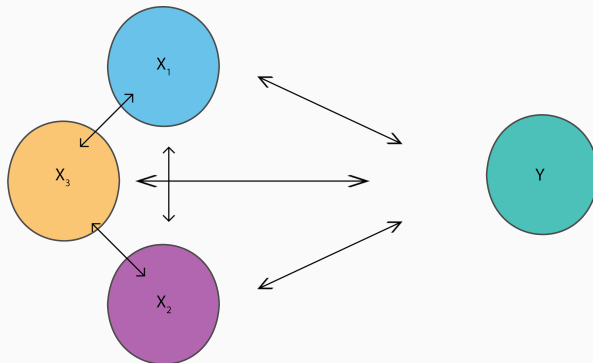
With three parameters, there are 6 relationship that are possible

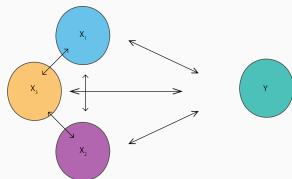… and it only gets worse as you add more parameters

The challenge is that only some of the
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Relationships between the predictors introduce the problem of collinearity
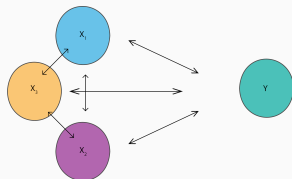
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In other words, parameter values for collinear predictors can't be trusted, which means we can't trust any of the predictions that the model makes.

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$$\text{temperature} = \beta_0 + \beta_1 \times \text{sunlight} + \varepsilon$$

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TEMP <- function(sun) {
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  sig <- 2
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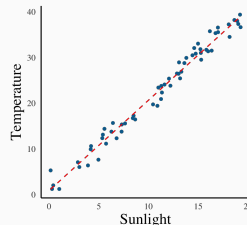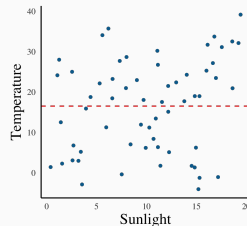
If the true relationship between sunlight, temperature, and plant mass is given by: $\mathrm{mass}_i = 0.25 \times \mathrm{temperature}_i + 1 \times \mathrm{sunlight}_i + \varepsilon_i$

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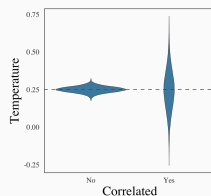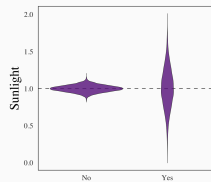
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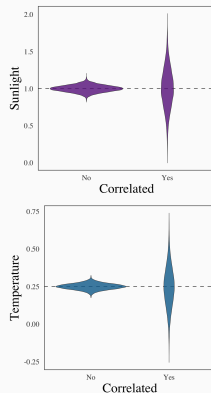data on parameter estimates:

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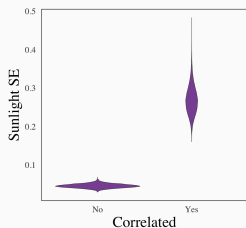
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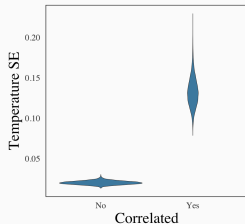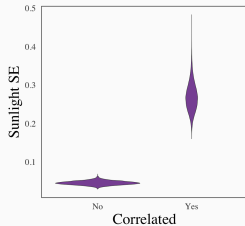

Note how some parameter estimates can even change signs!
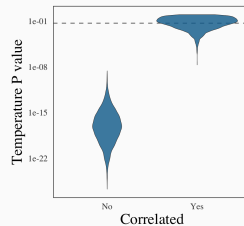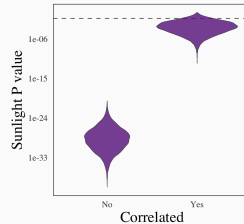
Collinearity also inflates standard errors
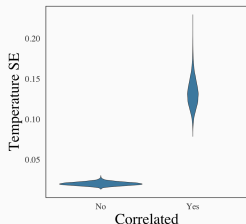
Collinearity also inflates standard errors

... which means that p values are untrustworthy

- Do nothing.

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- Collect more data.

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- Drop one of the correlated variables.

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- Perform a Principal Component Analysis (PCA) on the data to reduce dimensionality.

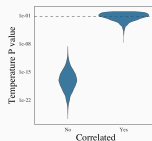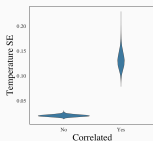Collinearity doesn't necessarily mean your model is incorrect

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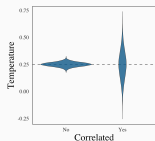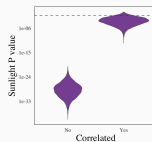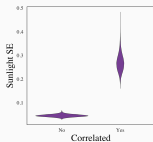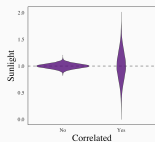
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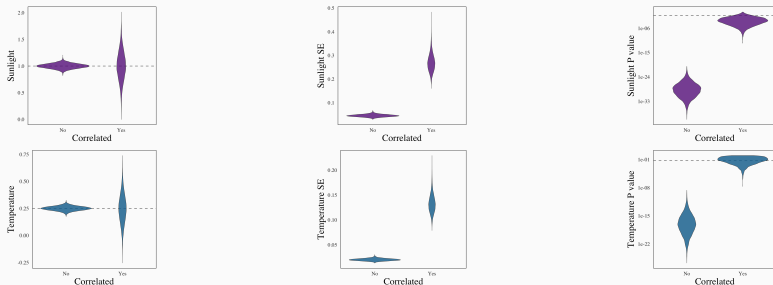
. . . but it does mean you need to be careful when making inferences.

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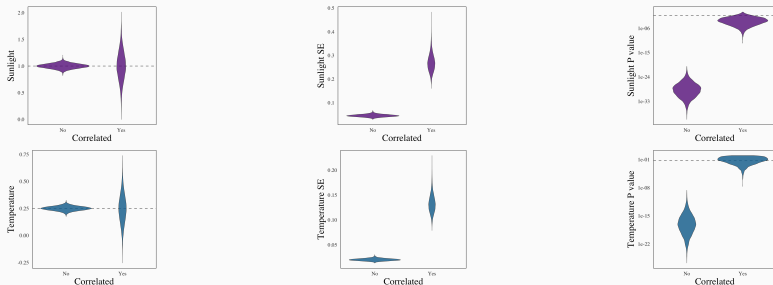
. . . but it does mean you need to be careful when making inferences.

Rule of thumb:: If the correlation between predictors is < 0.7 you won't run into major issues. Dormann et al. (2013). Collinearity: a review of methods to deal with it and a simulation study evaluating their performance. Ecography, 36(1), 27-46.

Collinearity doesn't necessarily bias the parameter estimates (i.e., parameter estimates are correct on average)

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With enough data, the problem of collinearity eventually goes away (terms asymptotic convergence).
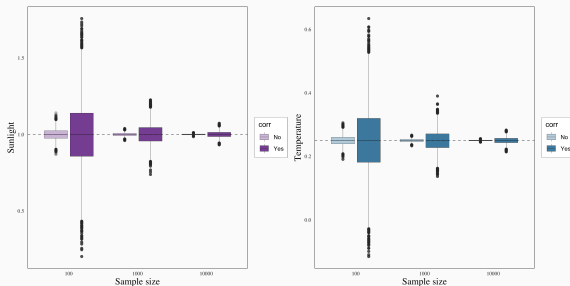
Dropping collinear parameters can correct for the issue of collinearity

Dropping collinear parameters can correct for the issue of collinearity, at a cost of reducing your R-squared

Dropping collinear parameters can correct for the issue of collinearity, at a cost of reducing your R-squared and potentially reducing biological relevance.

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We're not covering the details of PCAs, but, briefly, they reduce the dimensionality of a dataset by creating new uncorrelated variables that successively maximize variance.
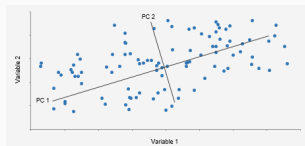
Source: statistiXL

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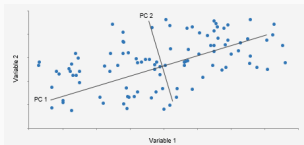
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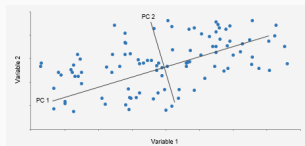
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Instead of fitting a model to your original data, you use the uncorrelated principal components in your analysis.

Analyses are robust to collinearity in the original data, but results can be more difficult to interpret.

Multiple linear regression in action

The Question: Do latitude and elevation have a measurable effect on ant species richness in forest plots in New England?

Gotelli, N.J. & Ellison, A.M. (2002). Biogeography at a regional scale: determinants of ant species density in bogs and forests of New England. Ecology, 83, 1604–1609

Number of Species	Latitude	Elevation
1.8	41.97	389
2.8	42	8
2.9	42.03	152
2.8	42.05	1
2.2	42.05	210
2.7	42.17	78
1.9	42.19	47
2.5	42.23	491
2.6	42.27	121
2.2	42.31	95
2.3	42.56	274
2.3	42.57	335
1.4	42.58	543
1.6	42.69	323
1.9	43.33	158
1.9	44.06	313
1.4	44.29	468
1.8	44.33	362
1.8	44.5	236
2.1	44.55	30
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1.8	44.5	236
2.1	44.55	30
1.8	44.76	353
1.8	44.95	133

Number of Species	Latitude	Elevation
1.8	41.97	389
2.8	42	8
2.9	42.03	152
2.8	42.05	1
2.2	42.05	210
2.7	42.17	78
1.9	42.19	47
2.5	42.23	491
2.6	42.27	121
2.2	42.31	95
2.3	42.56	274
2.3	42.57	335
1.4	42.58	543
1.6	42.69	323
1.9	43.33	158
1.9	44.06	313
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The relationships between richness, latitude, and elevation play out in multiple dimensions.
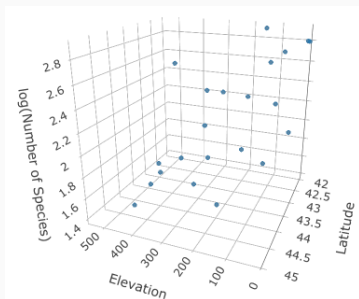
The relationships between richness, latitude, and elevation play out in
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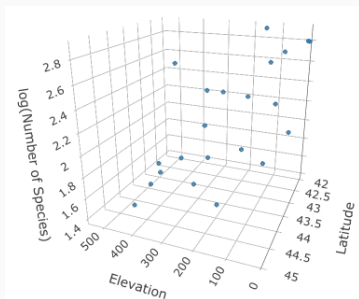
The first step is to check for any relationship between elevation and
latitude

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

```
data <- read.csv("Ant_Richness.csv")

preFIT <- lm(latitude ~ elevation, data = data)

summary(preFIT)
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Call:
lm(formula = latitude ~ elevation, data = data)

Residuals:
    Min      1Q  Median      3Q     Max
-1.2357 -0.7383 -0.5589  0.9789  2.0485

Coefficients:
             Estimate Std. Error t value Pr(>t)
(Intercept) 42.743402   0.411929 103.764  <2e-16 ***
elevation    0.001189   0.001461   0.814   0.425
---

Residual standard error: 1.091 on 20 degrees of freedom
Multiple R-squared:  0.03205,    Adjusted R-squared:  -0.01635
F-statistic: 0.6622 on 1 and 20 DF,  p-value: 0.4254
```
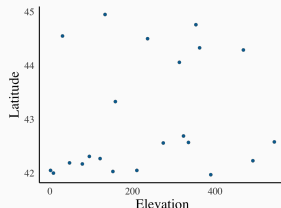
There was no significant relationship between our two predictors (Elevation and Latitude) so we can continue with our analyses.

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The regression problem in matrix notation is:

$$\begin{pmatrix} 1.8 \\ 2.8 \\ \vdots \\ 1.8 \end{pmatrix} = \begin{pmatrix} 1 & 41.97 & 389 \\ 1 & 42.00 & 8 \\ \vdots & \vdots & \\ 1 & 44.95 & 133 \end{pmatrix} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

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Because the dimensions of the matrices are all compatible we can estimate the parameters values using $\beta = (x^\mathsf{T} x)^{-1} x^\mathsf{T} y$.

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```r
x <- matrix(c(rep(1, nrow(data)),
              data$latitude,
              data$elevation),
            nrow = nrow(data), ncol = 3)

y <- matrix(data$num_sp,
            nrow = nrow(data), ncol = 1)

xtx <- t(x) %*% x
xtx.inv <- solve(xtx)
xty <- t(x) %*% y

beta <- xtx.inv %*% xty

beta

            [,1]
[1,] 11.115818937
[2,] -0.201828913
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lm(formula = num_sp ~ latitude + elevation, data = data)

Residuals:
     Min       1Q   Median       3Q      Max
-0.63613 -0.21966  0.06166  0.17932  0.58149

Coefficients:
              Estimate Std. Error t value Pr(>t)
(Intercept) 11.1158189  2.7445783   4.050 0.000683 ***
latitude    -0.2018289  0.0641510  -3.146 0.005318 **
elevation   -0.0013729  0.0004259  -3.223 0.004473 **
---

Residual standard error: 0.3131 on 19 degrees of freedom
Multiple R-squared:  0.5653,   Adjusted R-squared:  0.5196
F-statistic: 12.36 on 2 and 19 DF,  p-value: 0.0003651
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Ant Richness: Analysis

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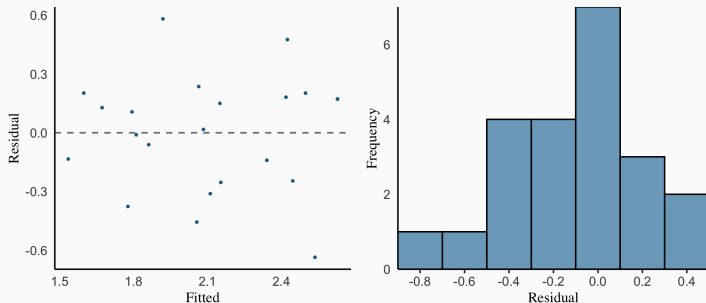
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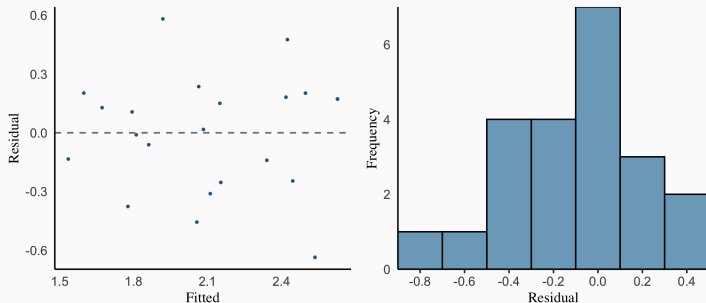
We'll cover residuals in more detail next lecture, but for now suffice it to say these look pretty good.

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It's important to be very careful when adding parameters to a model.

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set.seed(84)
NOISE <- rnorm(22)
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Residuals:
     Min       1Q   Median       3Q      Max
-0.47676 -0.09979 -0.03401  0.17771  0.41594

Coefficients:
             Estimate Std. Error t value Pr(>t)
(Intercept) 10.9552493  2.2723853    4.821 0.000137 ***
latitude    -0.1986631  0.0531102   -3.741 0.001497 **
elevation   -0.0014188  0.0003528   -4.021 0.000801 ***
NOISE       -0.1893679  0.0607058   -3.119 0.005922 **
---

Residual standard error: 0.2592 on 18 degrees of freedom
Multiple R-squared:  0.7179,   Adjusted R-squared:  0.6708
F-statistic: 15.27 on 3 and 18 DF,  p-value: 3.448e-05
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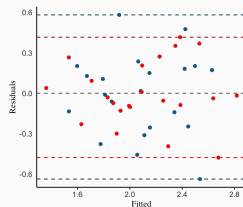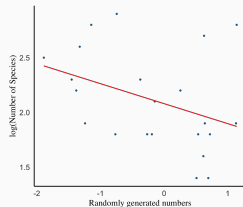

Our previous R^2 was ~0.57, so on the surface it looks like we have a better model, even though we know for a fact it's just junk.

Parameter Interactions

We opened today's lecture by noting that biological systems are complex with multiple variables influencing outcomes.

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Well, biological systems are complex, and variables can also interact with each other to influence outcomes (e.g., a breeze on a warm day is refreshing, a breeze in the middle of winter is not at all refreshing).

Interactions between explanatory variables are expressed as a product of the X's: $y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i} x_{2i} + \varepsilon_i$

For a model with two predictor variables and their interaction,

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i} x_{2i} + \varepsilon_i$$

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\qquad
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\qquad
x = \begin{pmatrix} 1 & x_1 1 & x_2 1 & x_1 1 x_2 1 \\ 1 & x_1 2 & x_2 2 & x_1 2 x_2 2 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_1 n & x_2 n & x_1 n x_2 n \end{pmatrix}
$$

Parameter Interactions in Action

The Question: We saw that latitude and elevation had a measurable effect on ant species richness. But what about the interaction between these?

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It's conceivable that high elevation at high latitude is worse for ants than high elevation at lower latitudes.

Source: WallpaperAccess

Source: Wikipedia

We can easily model interaction terms using the : operator:

```
FIT <- lm(num_sp ~ latitude + elevation + latitude:elevation, data = data)

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FIT <- lm(num_sp ~ latitude + elevation + latitude:elevation, data = data)
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```
Call:
lm(formula = num_sp ~ latitude * elevation, data = data)

Residuals:
     Min      1Q   Median      3Q     Max
-0.64627 -0.22755  0.07892  0.17200  0.60449

Coefficients:
                    Estimate Std. Error t value Pr(>t)
(Intercept)       12.2599423  5.1337948   2.388   0.0281 *
latitude          -0.2286208  0.1201511  -1.903   0.0732 .
elevation         -0.0064539  0.0190732  -0.338   0.7390
latitude:elevation 0.0001186  0.0004451   0.266   0.7929
---

Residual standard error: 0.3211 on 18 degrees of freedom
Multiple R-squared:  0.567,  Adjusted R-squared:  0.4949
F-statistic: 7.858 on 3 and 18 DF,  p-value: 0.001471
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Ant Richness: Analysis

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(Intercept)       2.499e+00  1.402e-01  17.826 9.6e-14 ***
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FIT2 <- lm(num_sp ~ latitude*elevation, data = data)
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A note on interactions in R

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. . . and always use objective measures to decide on what parameters should be included/discarded.