Extending linear regression

Adding more variables, transformations, and interactions

Diogo Melo - 28/01/2025

Linear regression is flexible!

Adding flexibility to our models

- The linear model we are using consists of making the parameters of probability distributions change according to some function
- The simplest function is a linear function

$$y_i \sim N(\mu_i, \sigma)$$
$$\mu_i = \alpha + \beta x_i$$

- Sometimes the relation between parameters and predictors is not linear
- We can use whatever functional shape we like, but it is useful to use transformations to linearize the relation

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Some simple transformations

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$$log(y_i) \sim N(\mu_i, \sigma)$$
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Log transforming the response

Multiplicative increments

- The log transformation of the response is a common transformation when the effect of the predictor on the response is thought to be multiplicative
  - A change of a unit in x is associated with a constant **percentage** change in y
- Many processes benefit from log transformation
  - Growth is proportional do previous size
  - Any multiplicative process

$$y_i \sim N(\mu_i, \sigma)$$
$$\mu_i = \alpha + \beta x_i$$
$$\downarrow$$
$$\Delta y \approx \beta \Delta x$$

$$log(y_i) \sim N(\mu_i, \sigma)$$
$$\mu_i = \alpha + \beta x_i$$
$$\downarrow$$
$$\% \, \Delta y \approx (100 \times \beta) \Delta x$$

Houle, D., Pélabon, C., Wagner, G. P. & Hansen, T. F. Measurement and meaning in biology. Q. *Rev. Biol.* 86, 3–34 (2011).

Biomass by diameter

Example of non-linear relation

Option 1: log-transform y

```
df = data.frame(diameter, biomass)
stan_fit = stan_glm(log(biomass) ~ diameter,
                    data = df)
```

Option A: Assign y a log-normal likelihood

```
rt_fit = ulam(alist(
            biomass ~ lognormal(mu, sigma),
            mu <- a + b*diameter,
            a ~ normal(0, 2),
            b ~ normal(0, 1),
            sigma ~ exponential(1)),
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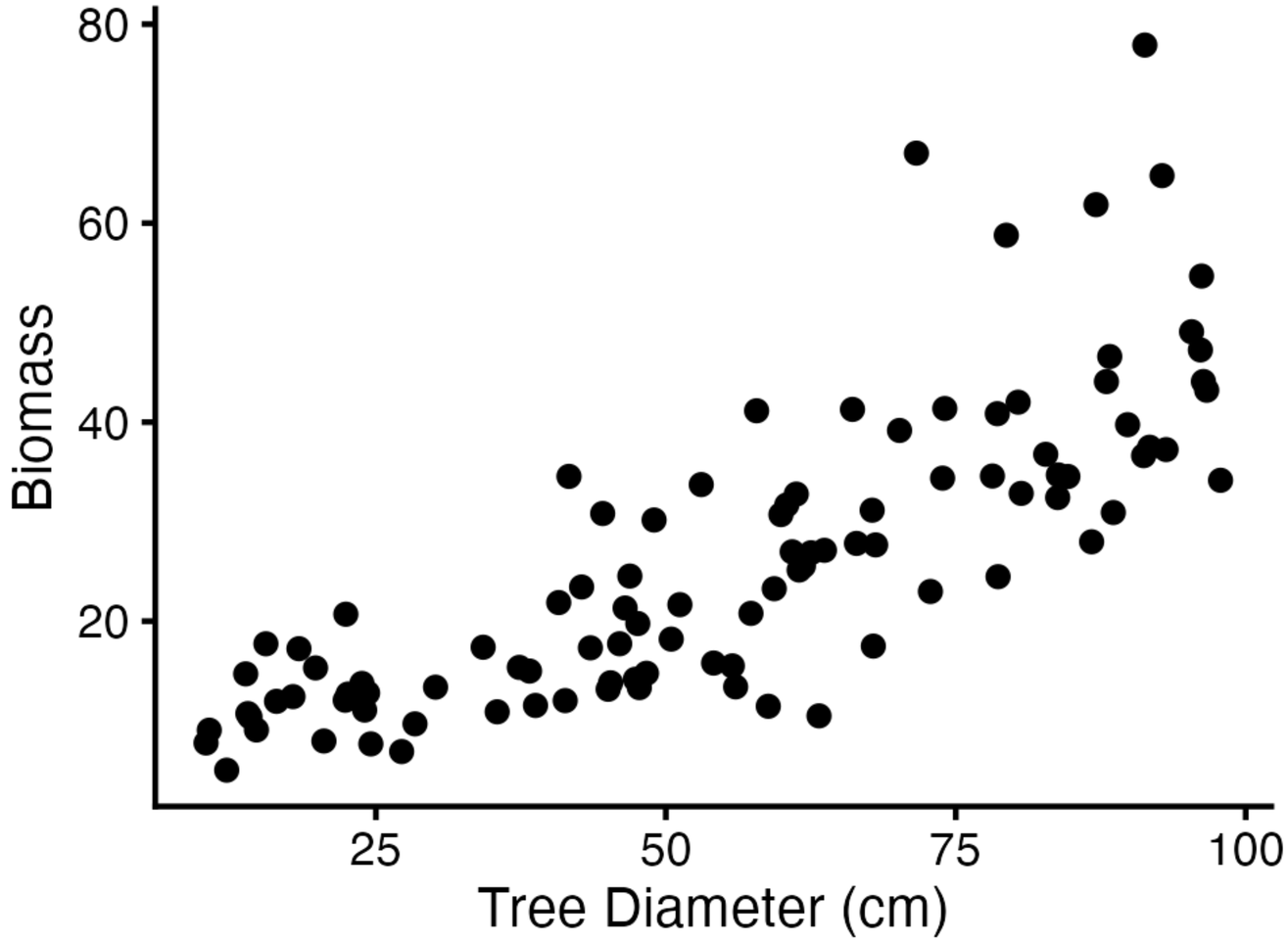

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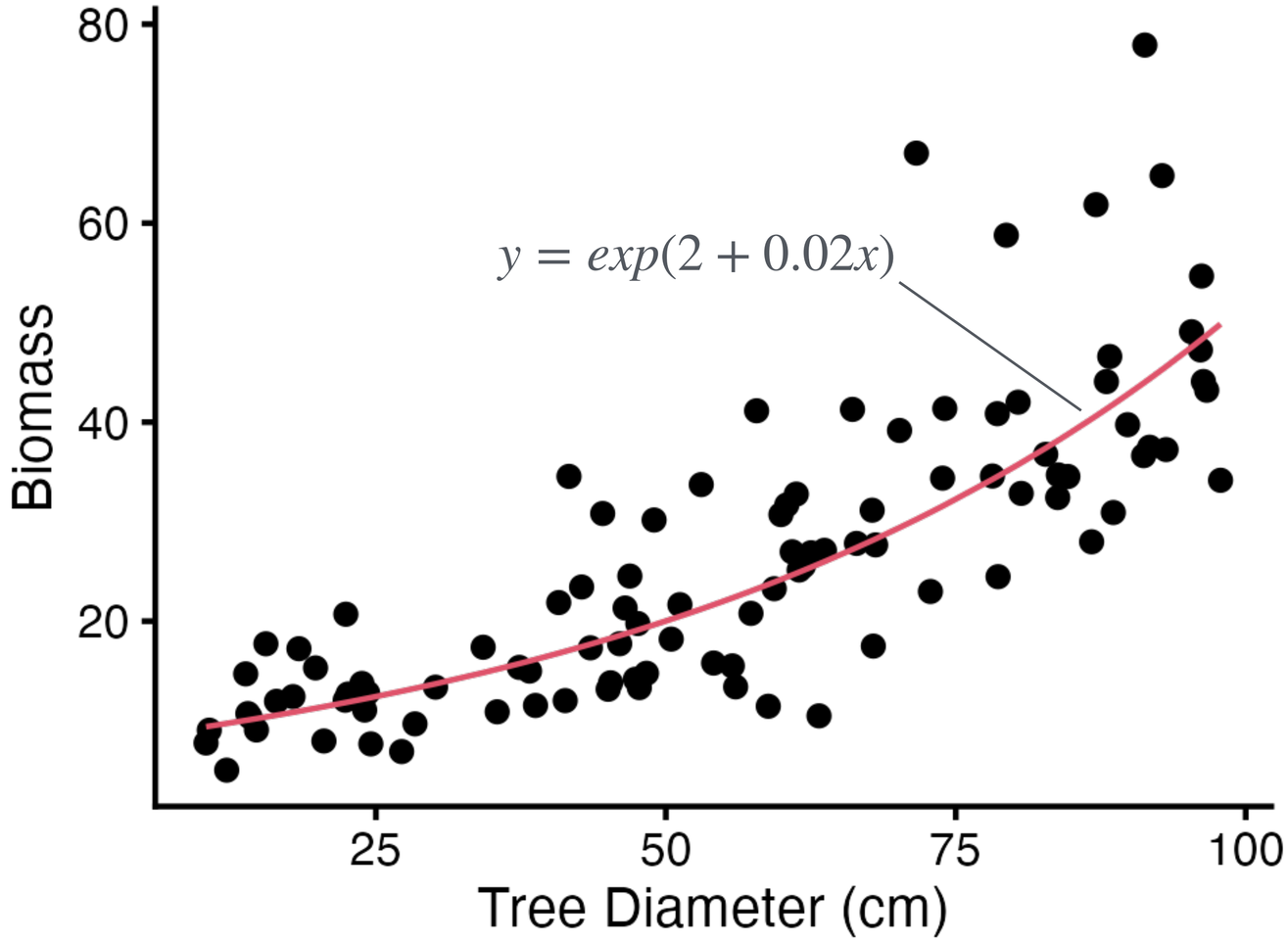

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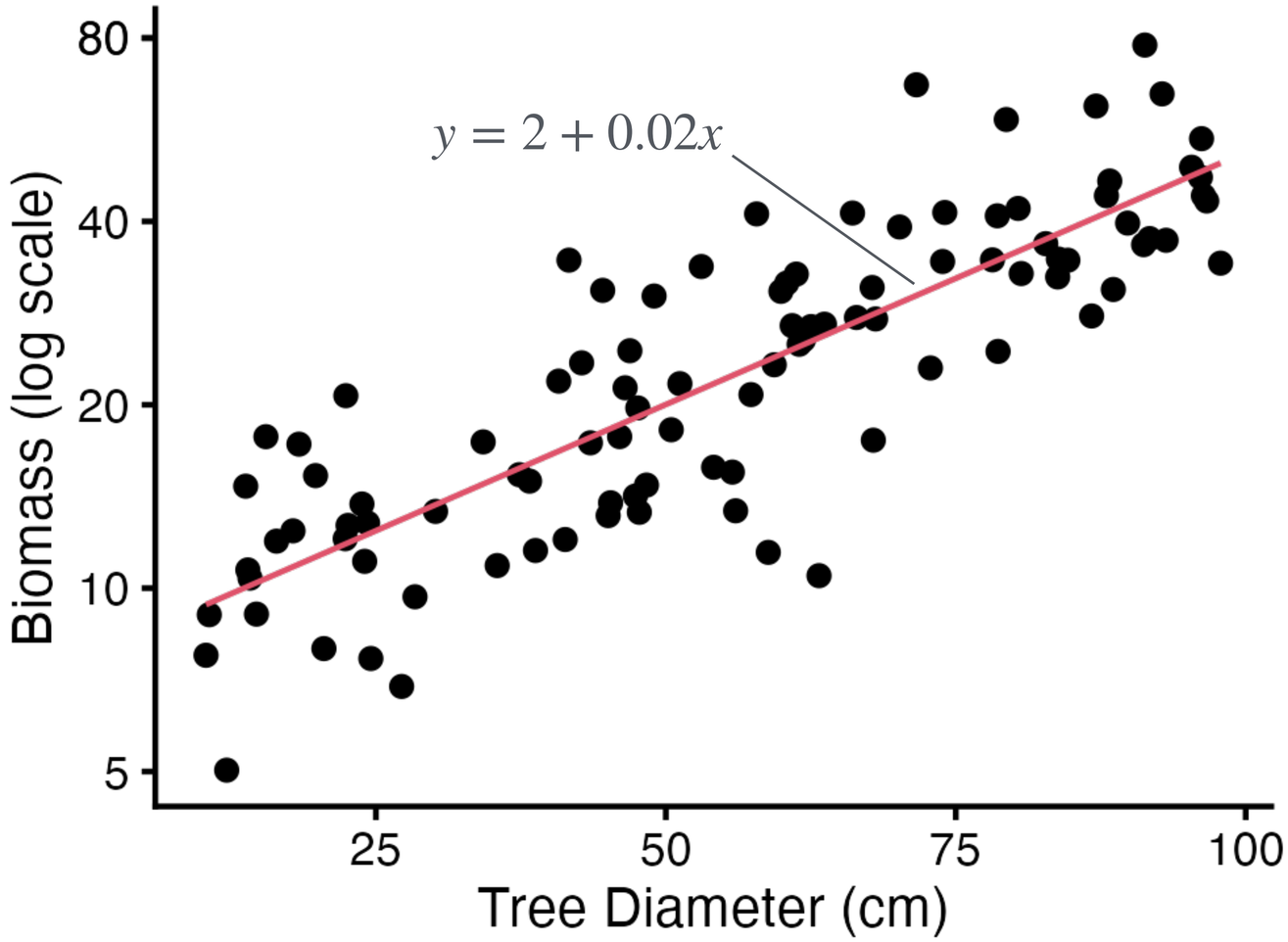


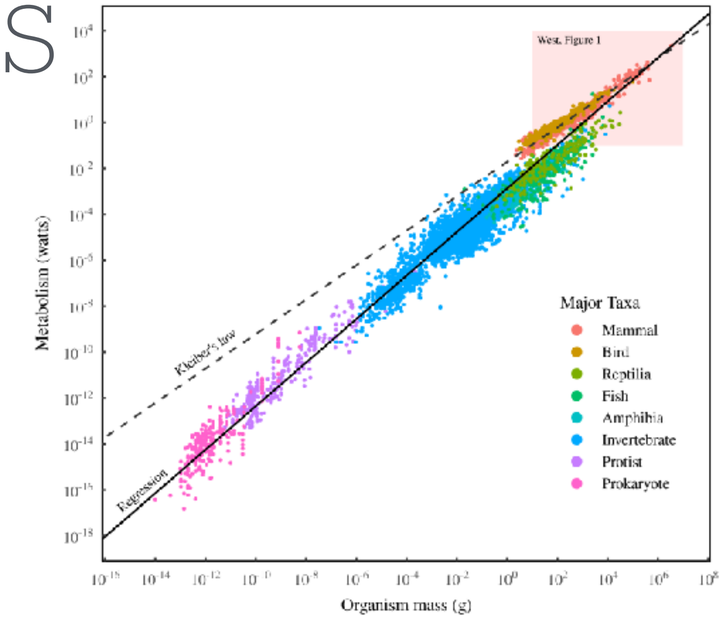
Power-law relations

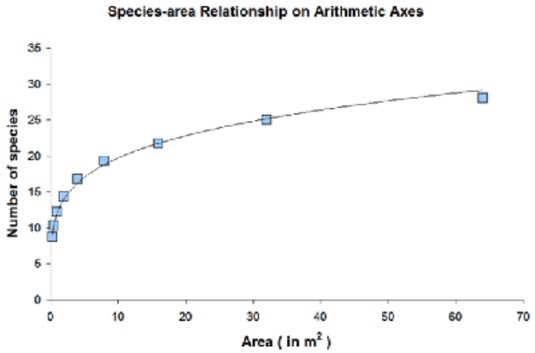
Log-log regressions

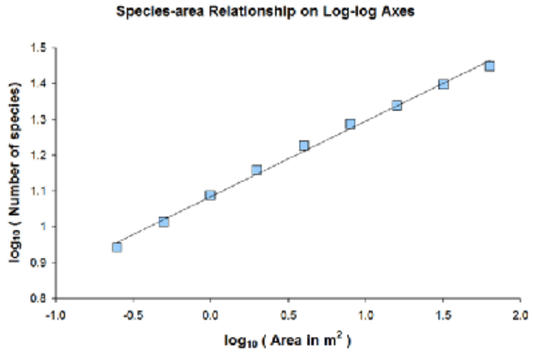
- Several biological relations take the form of power-law relations

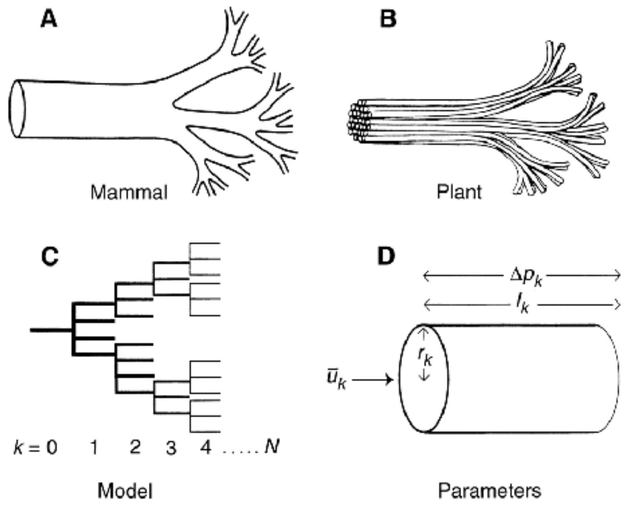
$$y \propto ax^b$$

- These appear for different reasons:
  - West et al. (1997) attempt to link scaling laws to fractal relations at different scales
  - Every time a proportional increase leads to a consistent proportional change (like in species-area relations)









West, G. B., Brown, J. H. & Enquist, B. J. A general model for the origin of allometric scaling laws in biology. *Science* **276**, 122–126 (1997).

Power-law relations

Log-log regressions

- Several biological relations take the form of power-law relations
- We can linearize these relations using a log-log transformation

$$y \propto ax^b$$

$$log(y) \propto log(ax^b) = log(a) + log(x^b) =$$

$$\boxed{log(y) \propto log(a) \ + \ b \ log(x)}$$

West, G. B., Brown, J. H. & Enquist, B. J. A general model for the origin of allometric scaling laws in biology. *Science* **276**, 122–126 (1997).

Power-law relations

Log-log regressions

- Several biological relations take the form of power-law relations
- We can linearize these relations using a log-log transformation
- In this model, the slope is and estimate of the exponent of the power-law
- The interpretation of the slope is that a 1% increase in x leads to a $\beta\,\%$ increase in y

$$log(y_i) \sim N(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta\ log(x_i)$$

$$\downarrow$$

$$\%\ \Delta y \approx \beta\,\%\ \Delta x$$

West, G. B., Brown, J. H. & Enquist, B. J. A general model for the origin of allometric scaling laws in biology. *Science* **276**, 122–126 (1997).

Quick reference for log transformations

Model	Dependent variable	Independent Variable	Interpretation of β
Level-level	y	x	$\Delta y \approx \beta \Delta x$
Level-log	y	log(x)	$\Delta y \approx (\frac{\beta}{100}) \% \Delta x$
log-level	log(y)	X	$\% \Delta y \approx (100\ \beta) \Delta x$
Log-log	log(y)	log(x)	$\% \Delta y \approx \beta \% \Delta x$

Linear regression is flexible!

We can modify our functions however we like

- The linear model we are using consists of making the parameters of probability distributions change according to some function

- The simplest function involves a single predictor and slope

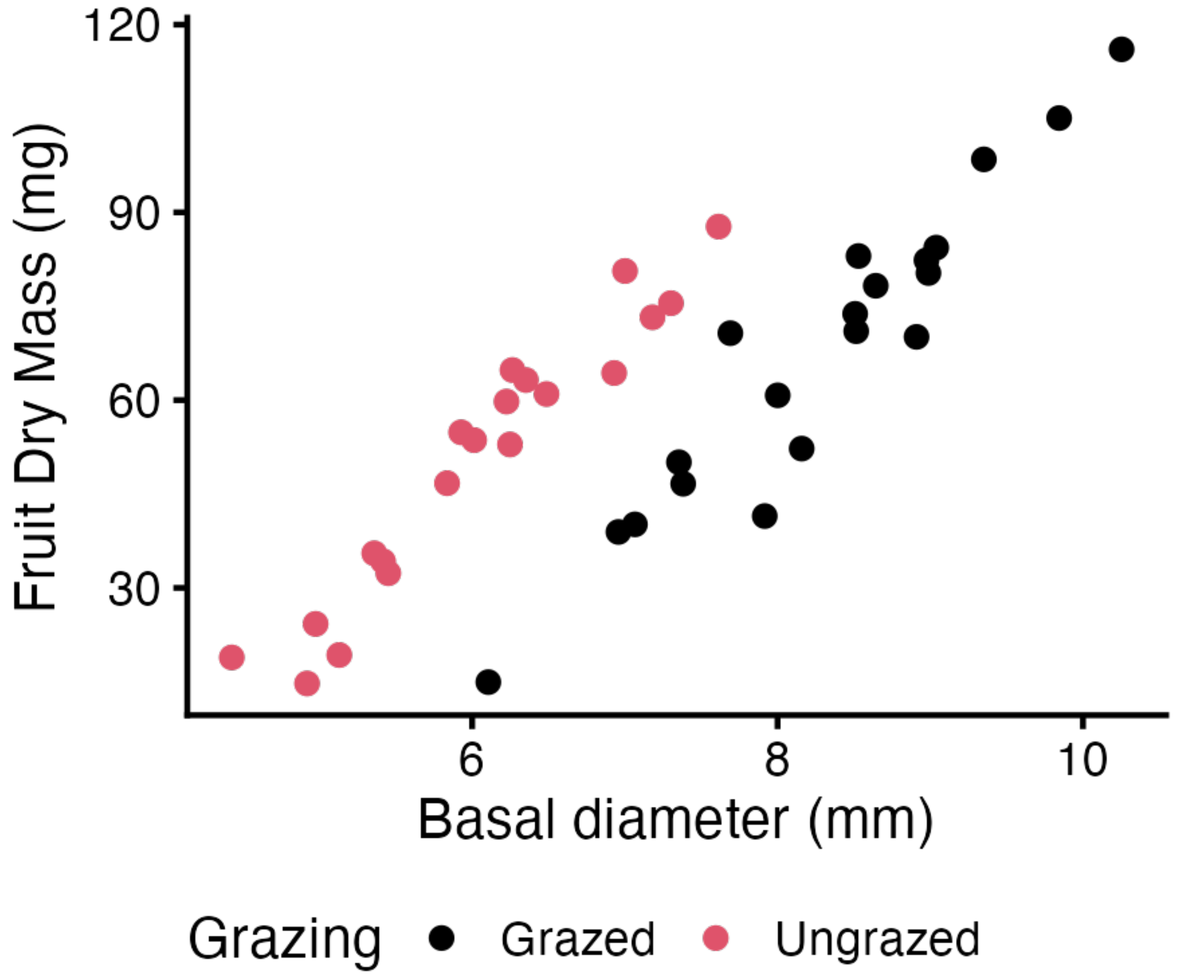
$$y_i \sim N(\mu_i, \sigma)$$
$$\mu_i = \alpha + \beta x_i$$

$$y_i \sim N(\mu_i, \sigma)$$
$$\mu_i = \alpha + \beta_1 x_{i1} + \beta_2 x_{i2}$$

- If we have more predictors, we can simply add them to the regression equation

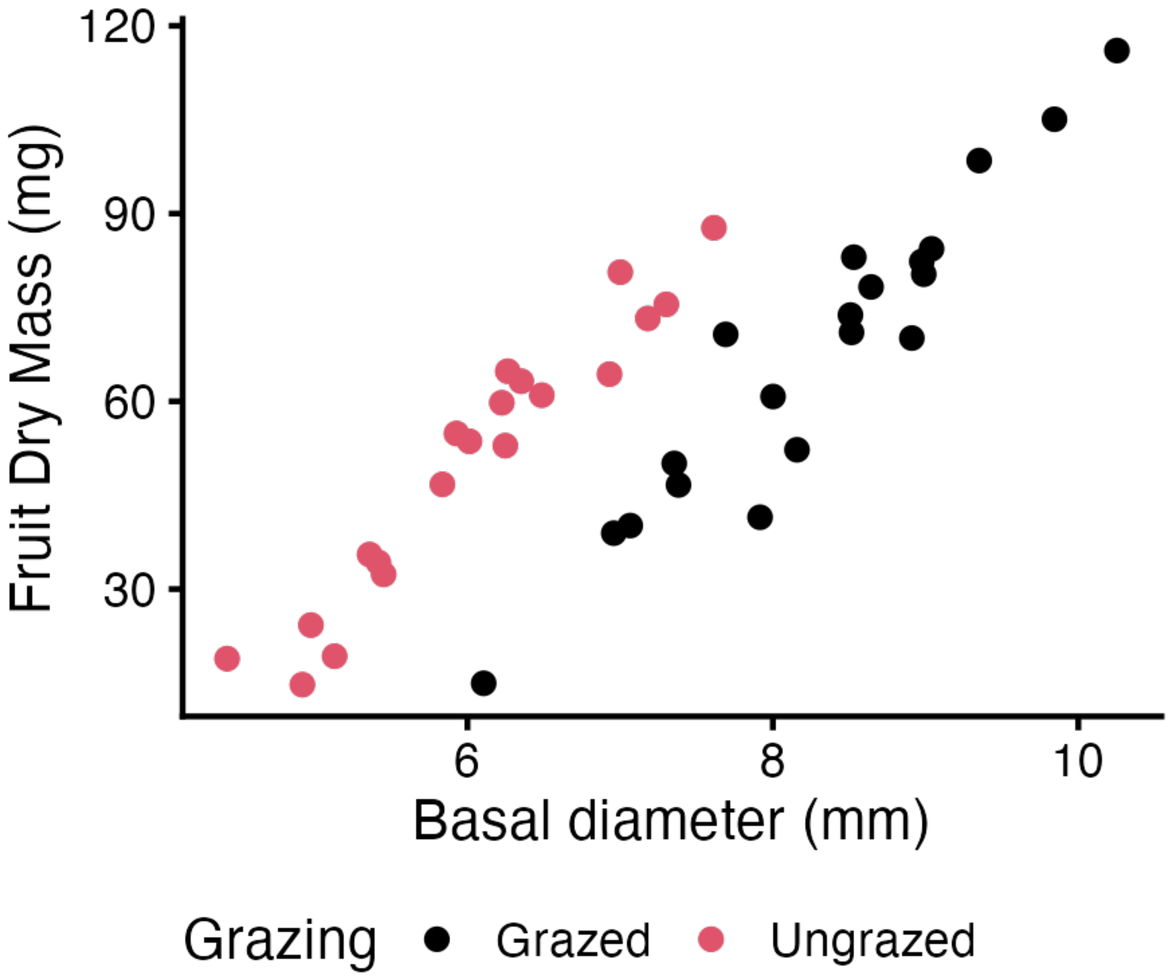
Example with more predictors

- **Question**: what's the impact of herbivory on plant fitness?
- **Field experiment**: 40 plants of *Ipomopsis agreggata* assigned at random to two treatments: unprotected from grazing by rabbits and protect from grazing by fenced cages.
- Response variable: fruit yield of each plant (mg dry mass)
- Predictor variables:
  - Treatment: fenced or non-fenced
  - Basal diameter of each plant (mm), measured before the treatment



Data from: Crawley (2007) The R Book

Scale variables



- It's good practice to scale variables by their standard deviation and subtract the mean:

$$\tilde{y}_i = \frac{y_i - \bar{y}}{sd(y)}$$

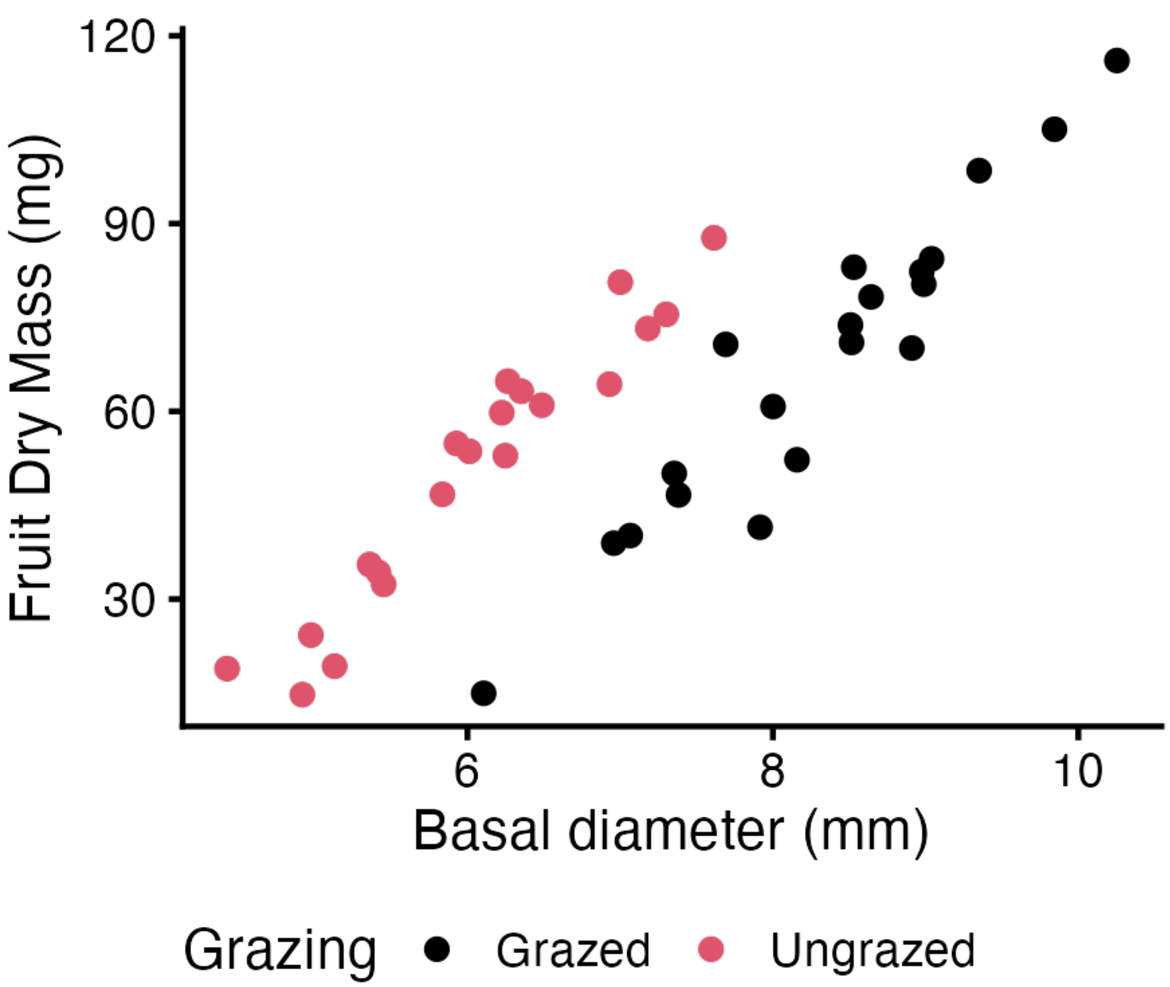
- The **z-score** of a continuous variable is a measure of how many standard deviations a data point is from the mean of the dataset

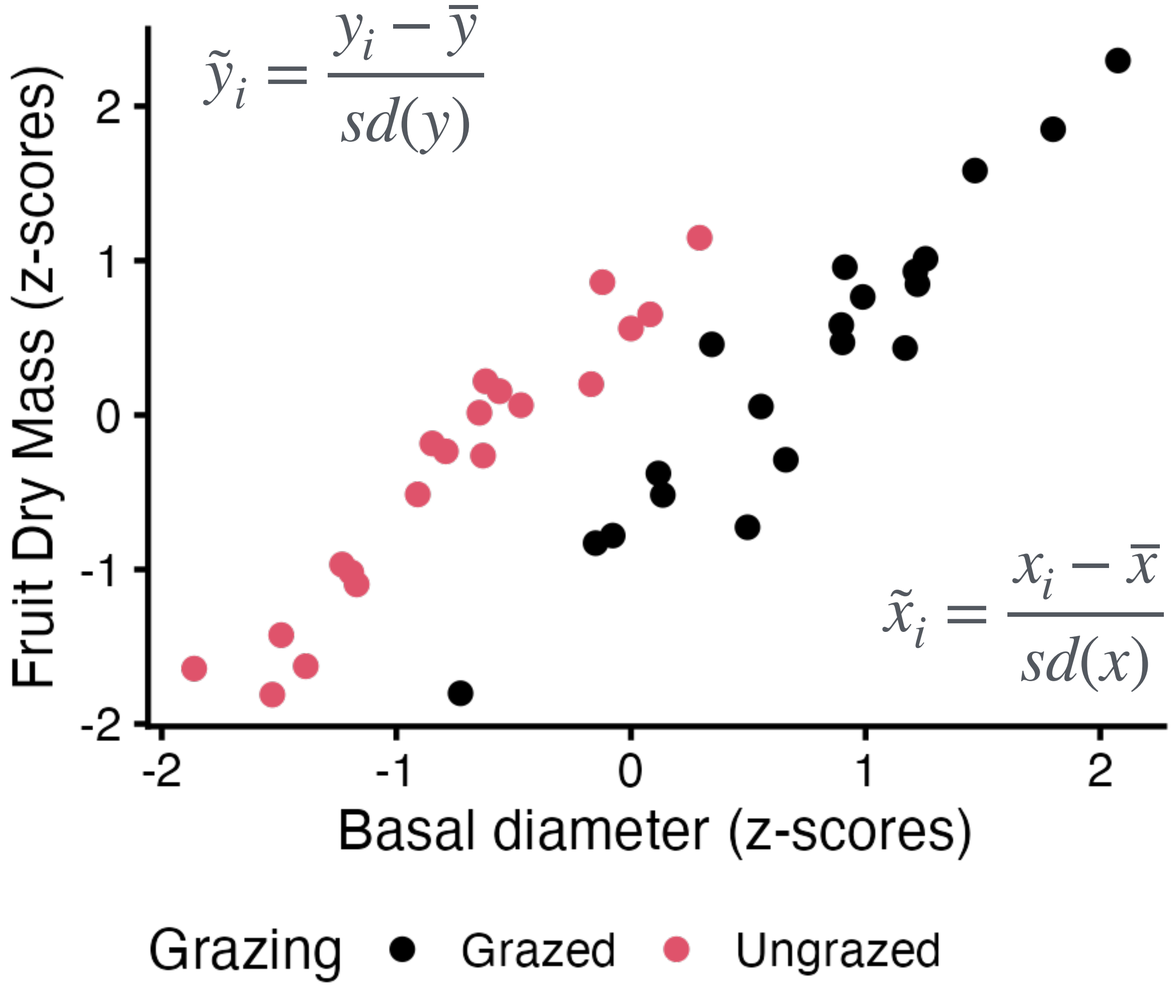
- Using z-scores makes coefficients easier to interpret and comparable across variables with different scales

- The transformation is linear, and we can always recover parameter values on their original scale by multiplying by the standard deviation

Scale variables

Using standard deviation units makes everything simpler





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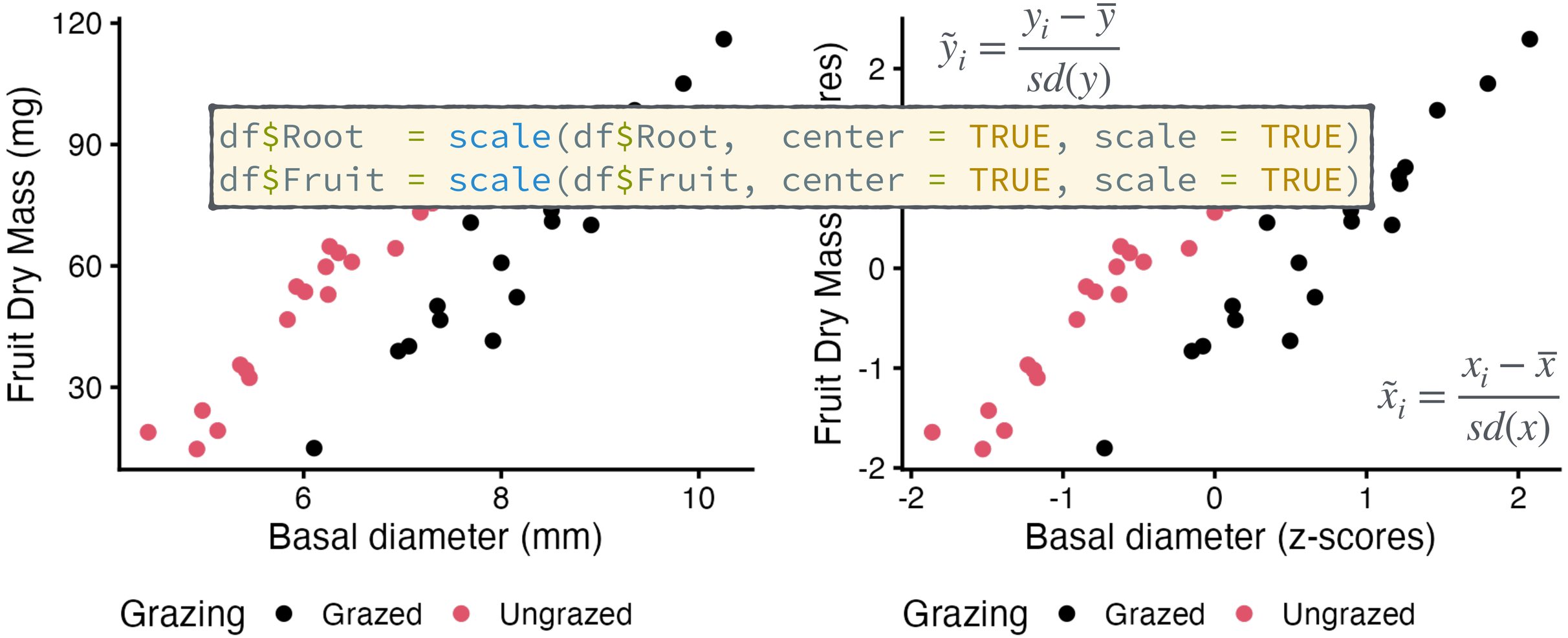
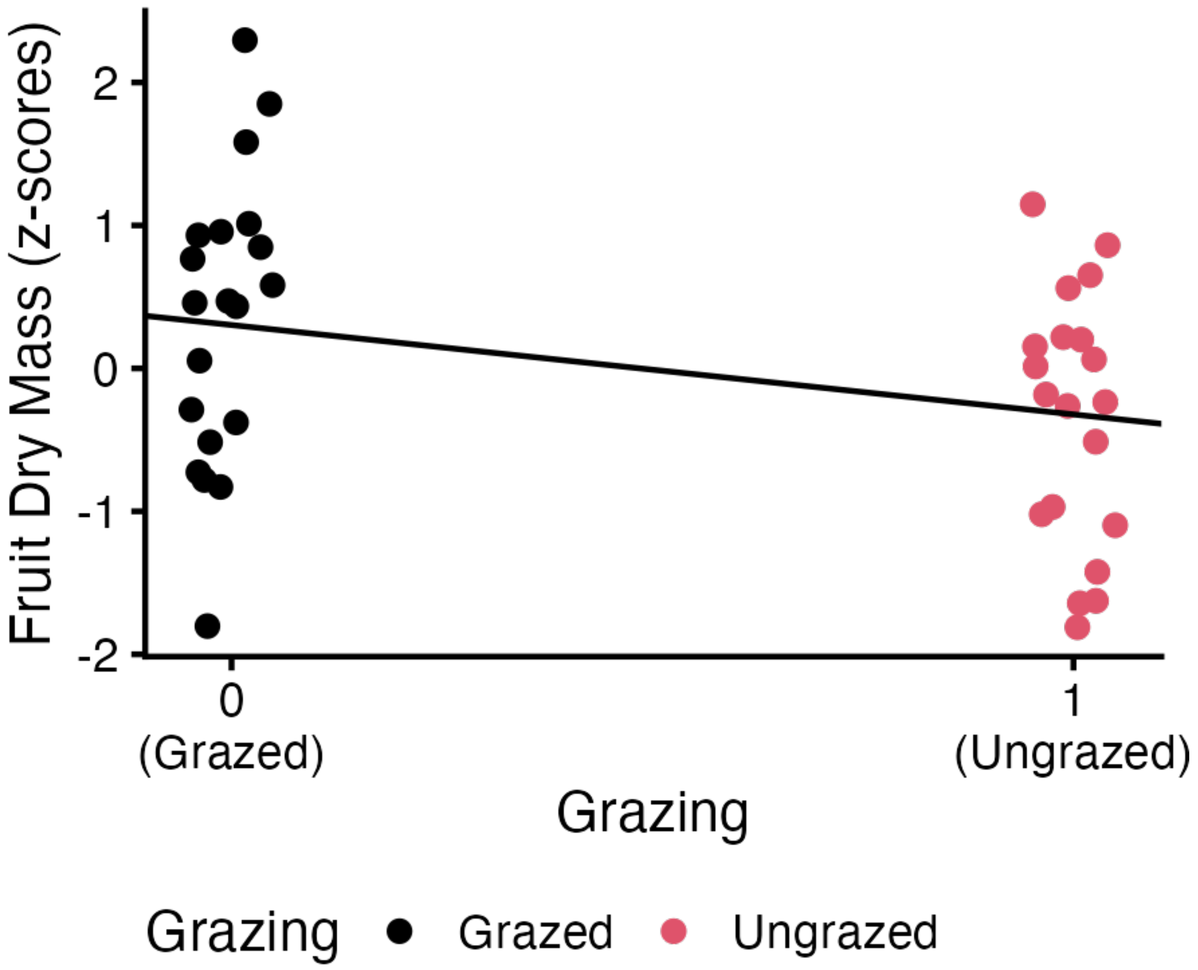


Model with only treatment

```
df$Grazing0 = ifelse(df$Grazing ==
"Ungrazed", 1, 0) # numeric coding

m1 = ulam(alist(Fruit ~ normal(mu, sigma),
            mu <- a + b*Grazing0,
            a ~ normal(0, 1),
            b ~ normal(0, 1),
            sigma ~ exponential(1)),
      data = df, chains = 4, cores = 4)
```

```
> precis(m1, prob = 0.95)
        mean   sd  2.5% 97.5%
a       0.32 0.21 -0.09  0.72
b      -0.66 0.30 -1.23 -0.06
sigma   0.97 0.12  0.77  1.22
```



Model with treatment and size

```
m2 = ulam(alist(
            Fruit ~ normal(mu, sigma),
            mu <- a + b*Grazing0 + c*Root,
            a ~ normal(0, 1),
            b ~ normal(0, 1),
            c ~ normal(0, 1),
            sigma ~ exponential(1)),
      data = df, chains = 4, cores = 4)
```

```
> precis(m2, prob = 0.95)
        mean   sd  2.5% 97.5%
a      -0.71 0.08 -0.86 -0.54
b       1.42 0.14  1.13  1.67
c       1.39 0.07  1.26  1.53
sigma   0.28 0.03  0.23  0.36
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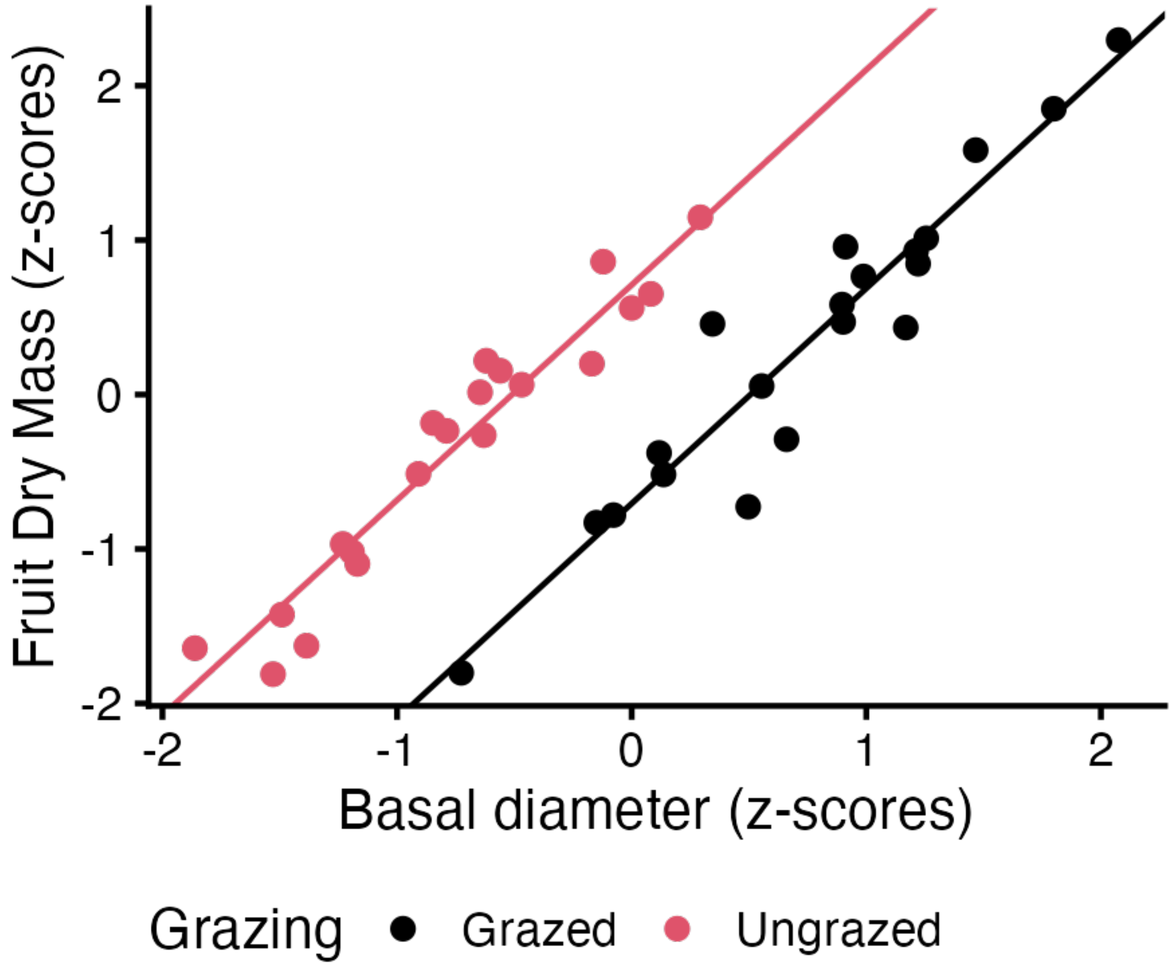

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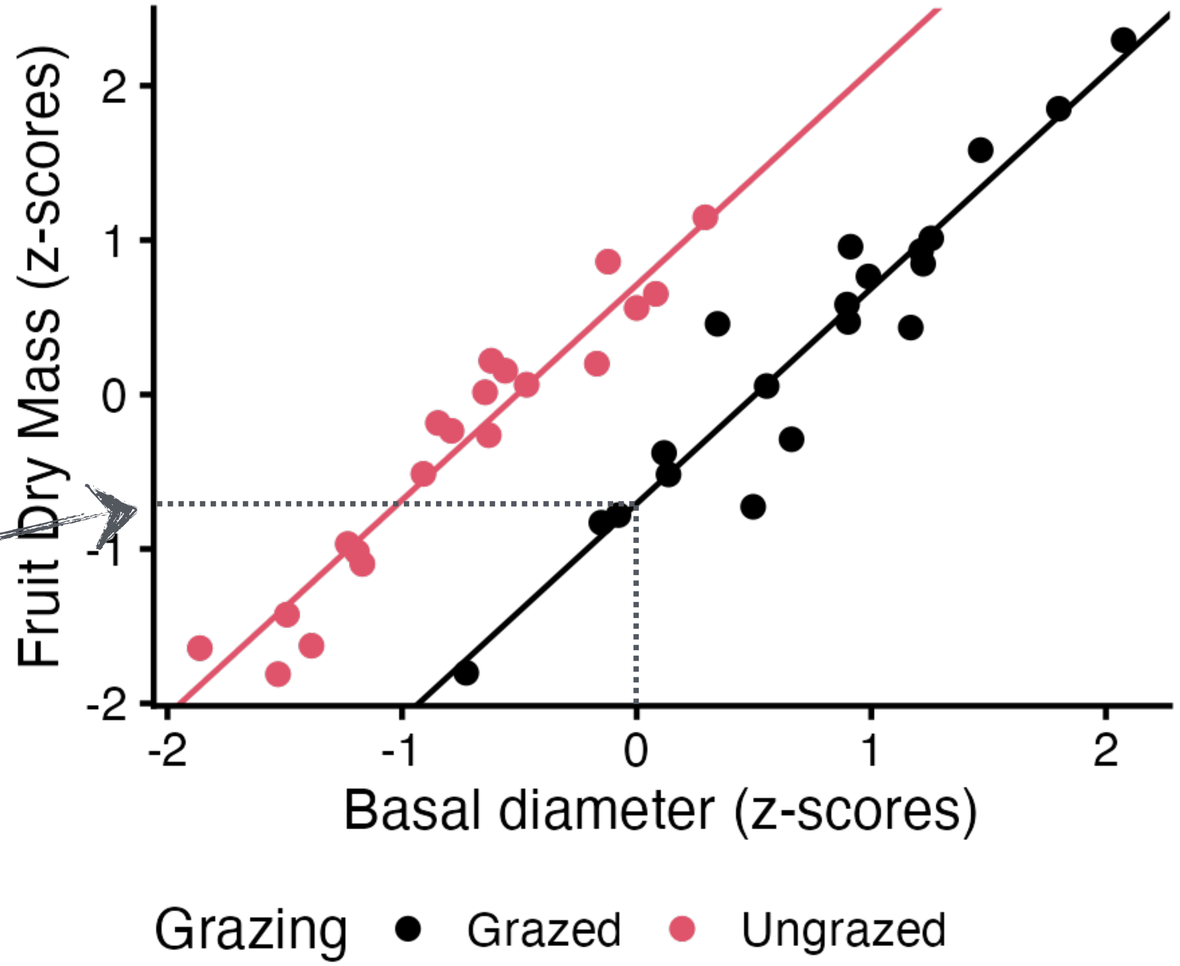

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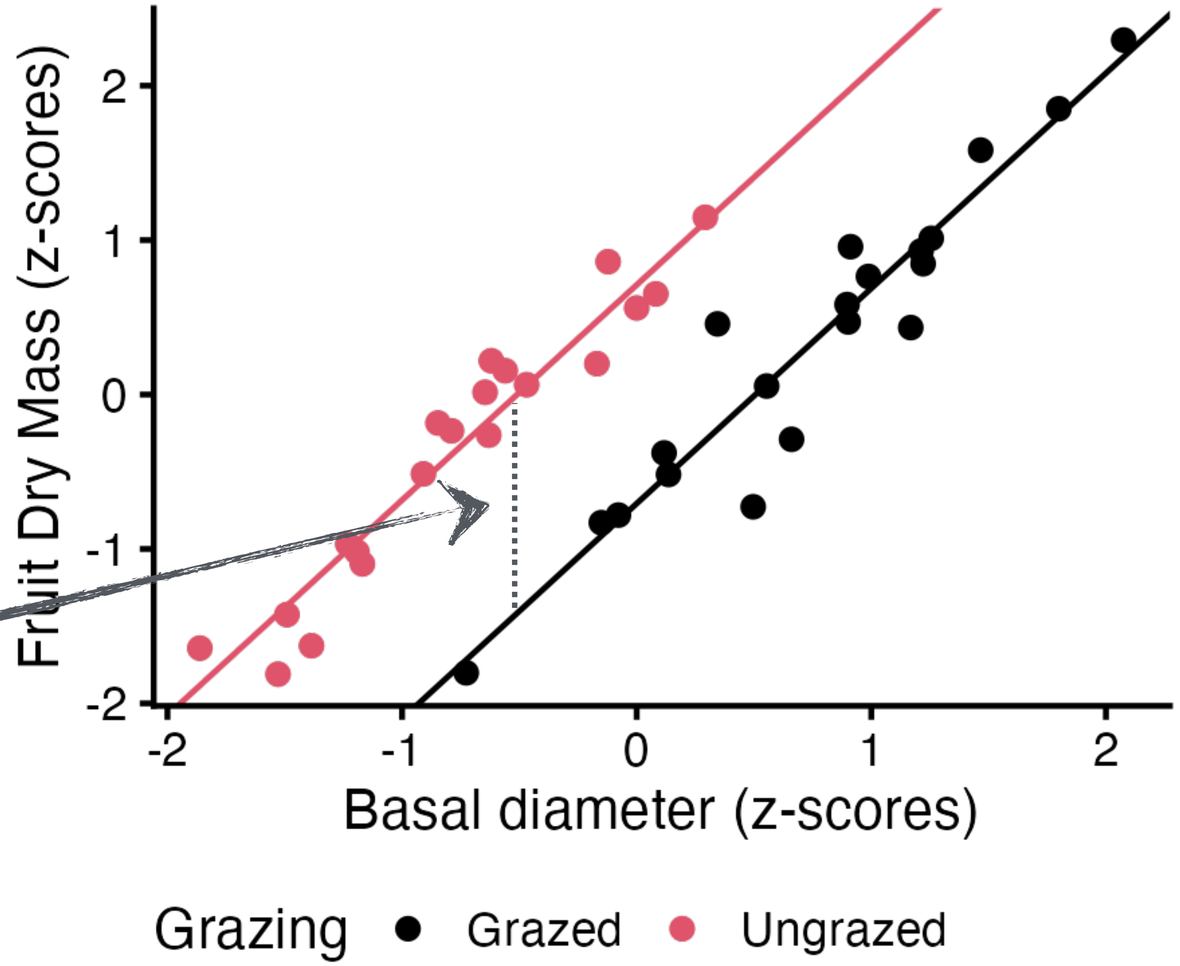

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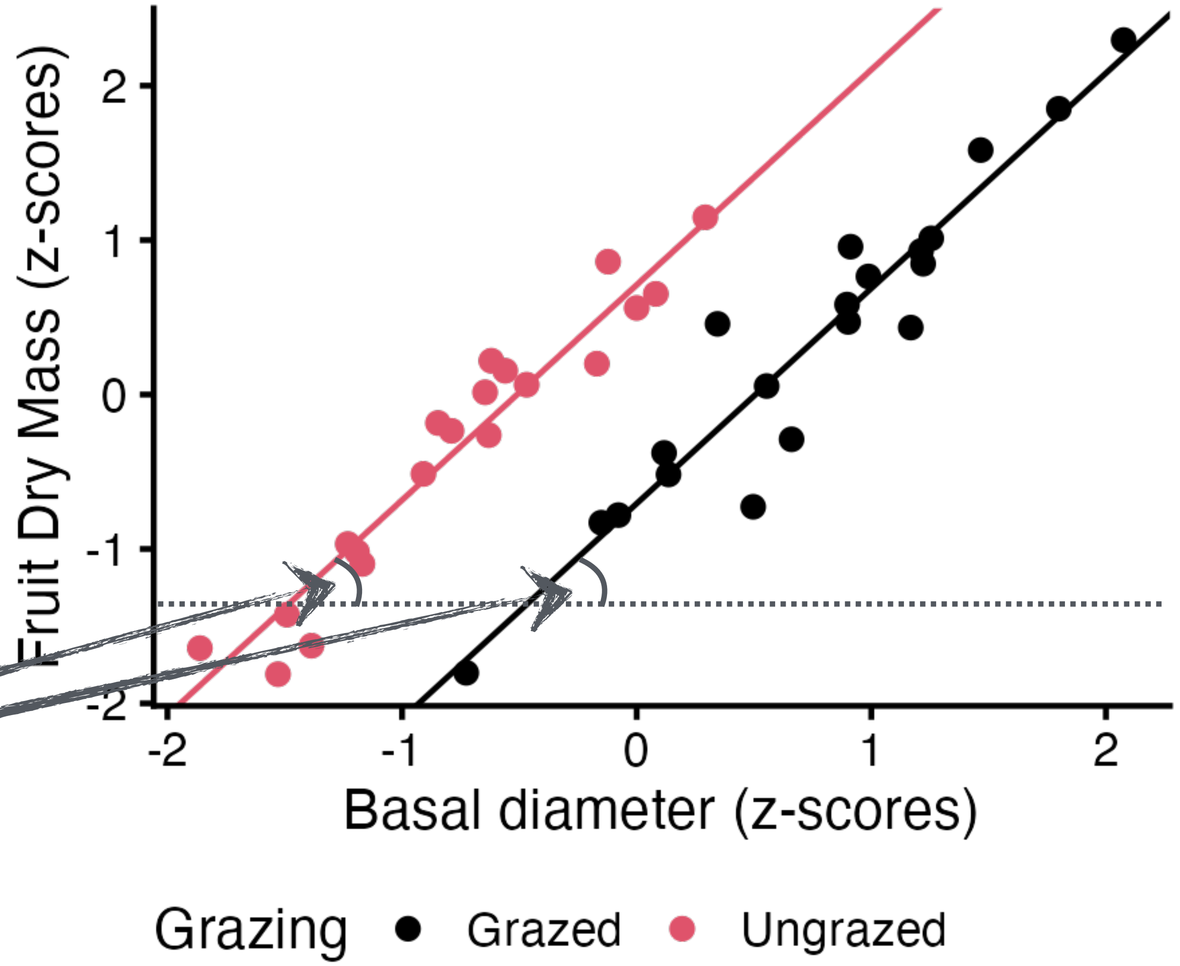
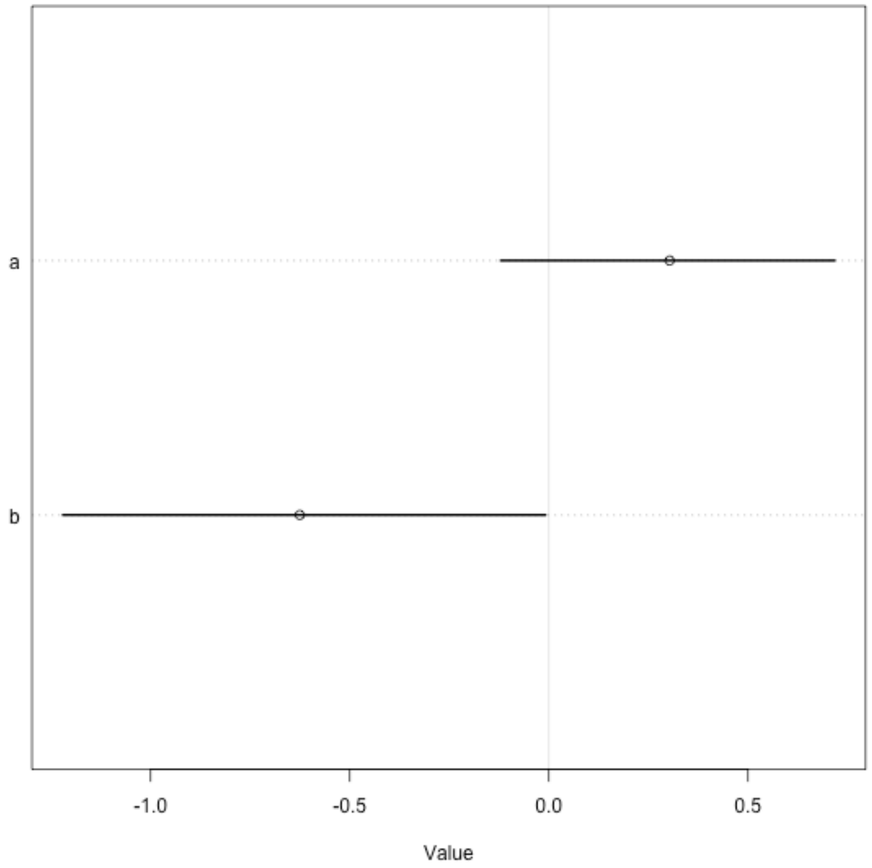


Comparing model estimates

$$y_i \sim N(\mu_i, \sigma)$$
$$\mu_i = \alpha + \beta x_i$$



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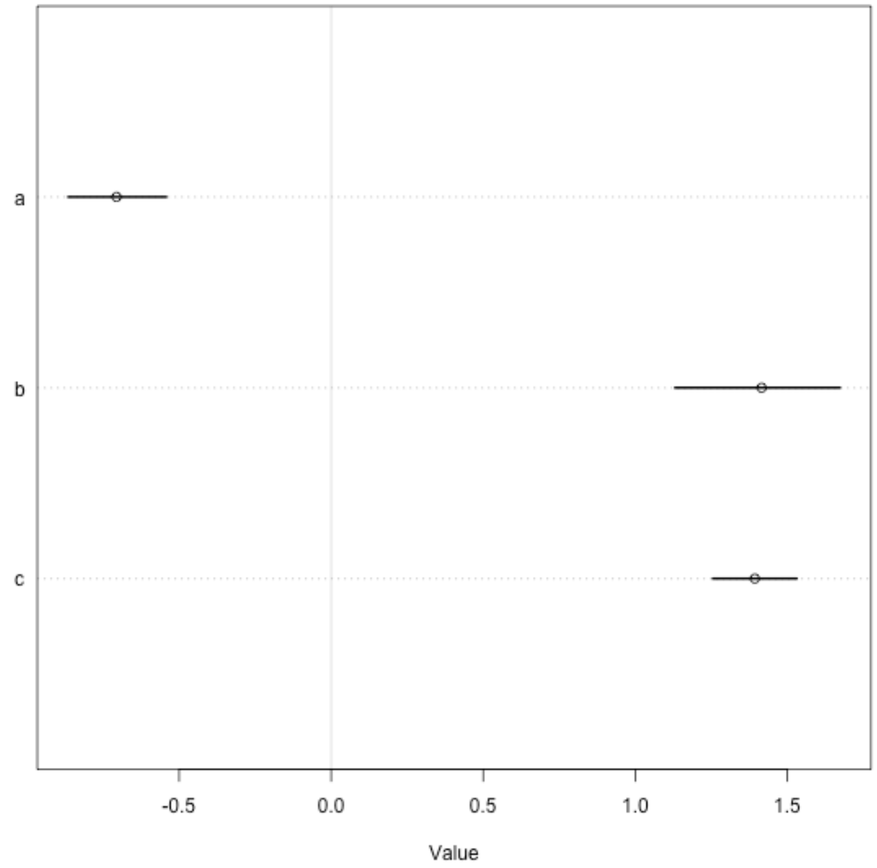


Why do the coefficients change?

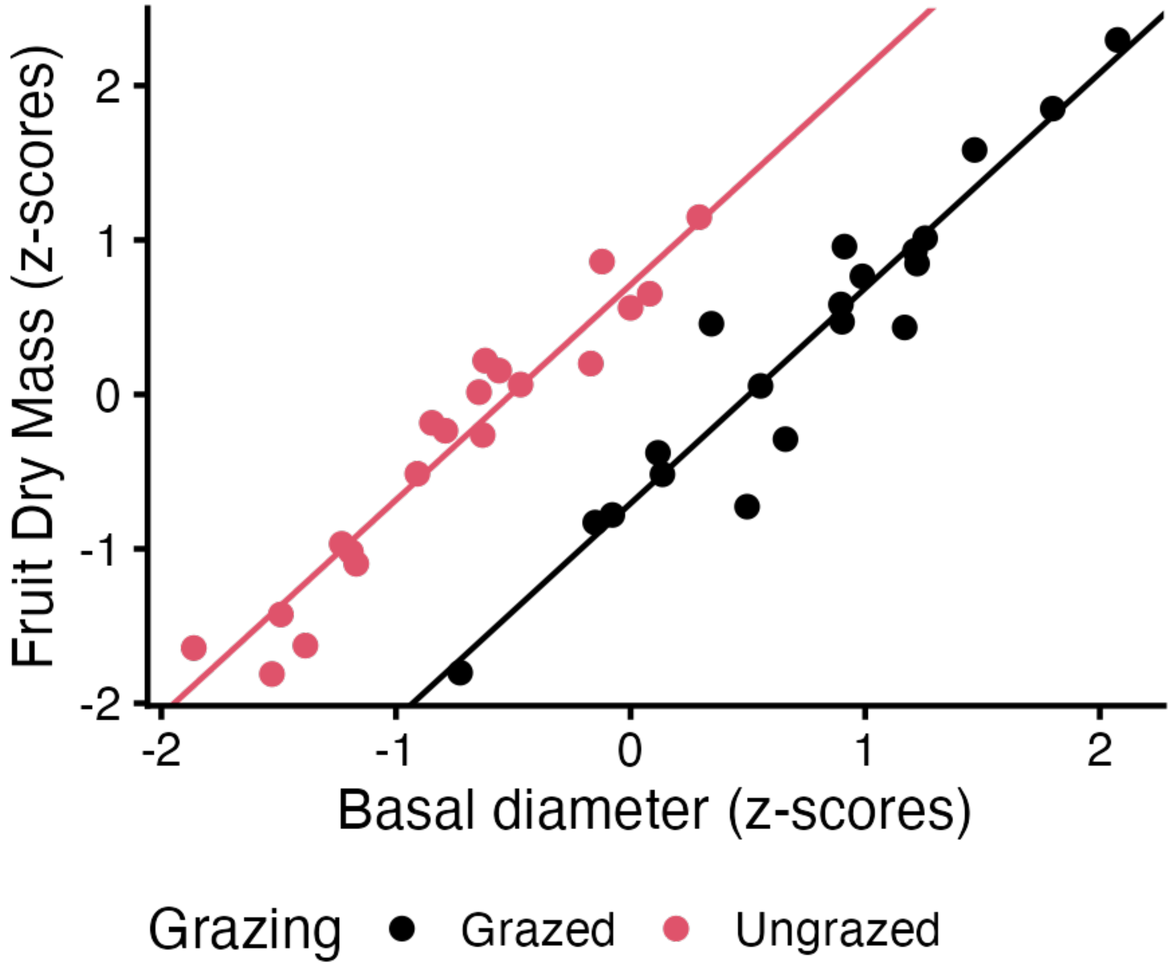
Multiple regression as control

- Coefficients are comparisons, and adding predictors to a regression has the same effect as **stratifying** the data

- The objetive of adding more predictors to a linear model is to compare **like-to-like**:

  1. What is the difference between treatments for plants of the same initial size?

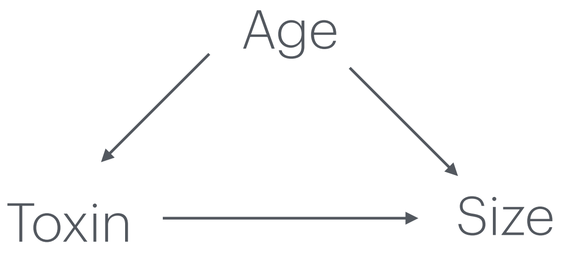
  2. What is the effect of initial size given a particular treatment?



Using simulations to understand multiple regression

- Simulations are a powerful tool to understand how these models behave
- **Use them liberally! Use them often!**
- Ask:
  - What is the data generating process of system?
  - What model represents this process?
- Simulate data under this model, try to fit the data

- Example:
  - **Question**: What is the effect of toxin exposure on the size of individuals in a population?
  - Age affects both toxin exposure and size



Using simulations to understand multiple regression

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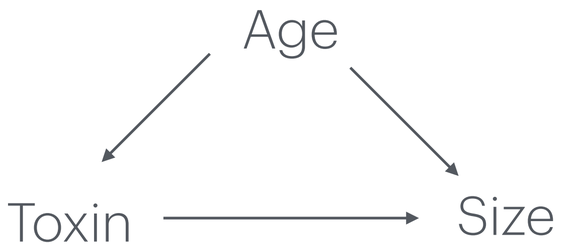
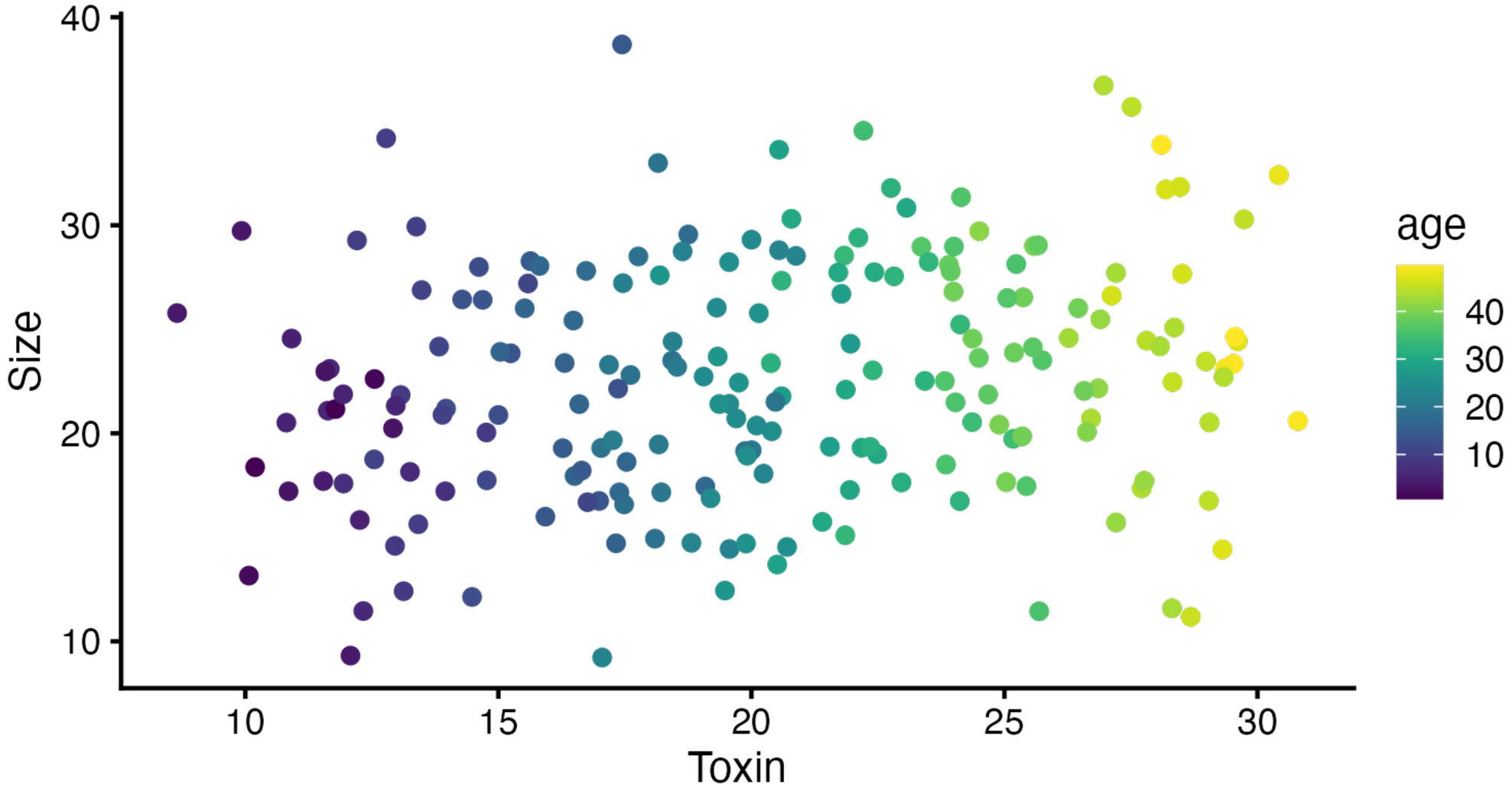


Possible model:

$$age_i = Uniform(0, 50)$$
$$toxin_i = Normal(10 + 0.4 \times age_i, 1)$$
$$size_i = Normal(30 - 1 \times toxin_i + 0.5 \times age_i, 5)$$

```
set.seed(1)
age <- runif(200, 0, 50)
toxin <- rnorm(200, 10 + 0.4*age, 1)
size = 30 - 1*toxin + 0.5*age + rnorm(200, 0, 5)
df = data.frame(age = age,
                toxin = toxin,
                size = size)
```

Simulated data



Center data and define model

```
df0 = df
df0$age   = scale(df0$age, scale = FALSE)
df0$toxin = scale(df0$toxin, scale = FALSE)
df0$size  = scale(df0$size, scale = FALSE)
```

$$size_i \sim Normal(\mu_i, \sigma)$$

$$\mu_i = a + b \times toxin_i + c \times age_i$$

```
rt_fit = ulam(alist(size ~ normal(mu, sigma),
            mu <- a + b*toxin + c*age,
            a ~ normal(0, 0.3),
            b ~ normal(0, 1),
            c ~ normal(0, 1),
            sigma ~ exponential(1)),
          data = df0, chains = 4, cores = 4)
```

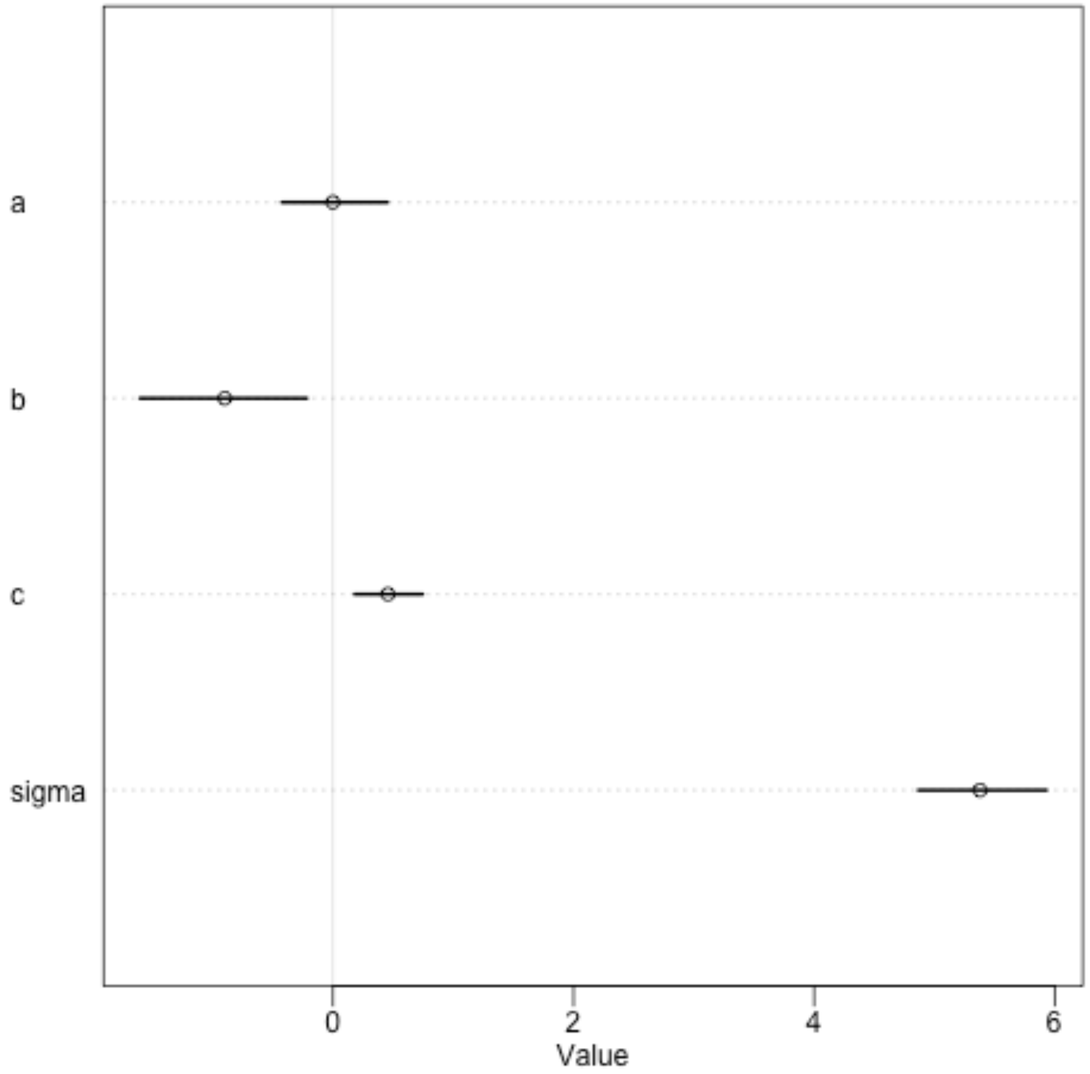
Model fit

$$size_i \sim Normal(\mu_i, \sigma)$$

$$\mu_i = a + b \times toxin_i + c \times age_i$$

```
> precis(rt_fit, prob = 0.95)
       mean   sd  2.5% 97.5% rhat ess_bulk
a      0.00 0.22 -0.43  0.45    1  1679.38
b     -0.90 0.35 -1.60 -0.22    1   821.89
c      0.46 0.14  0.18  0.74    1   791.07
sigma  5.38 0.27  4.87  5.93    1  1225.56

> plot(precis(rt_fit, prob = 0.95))
```



Estimates and true values

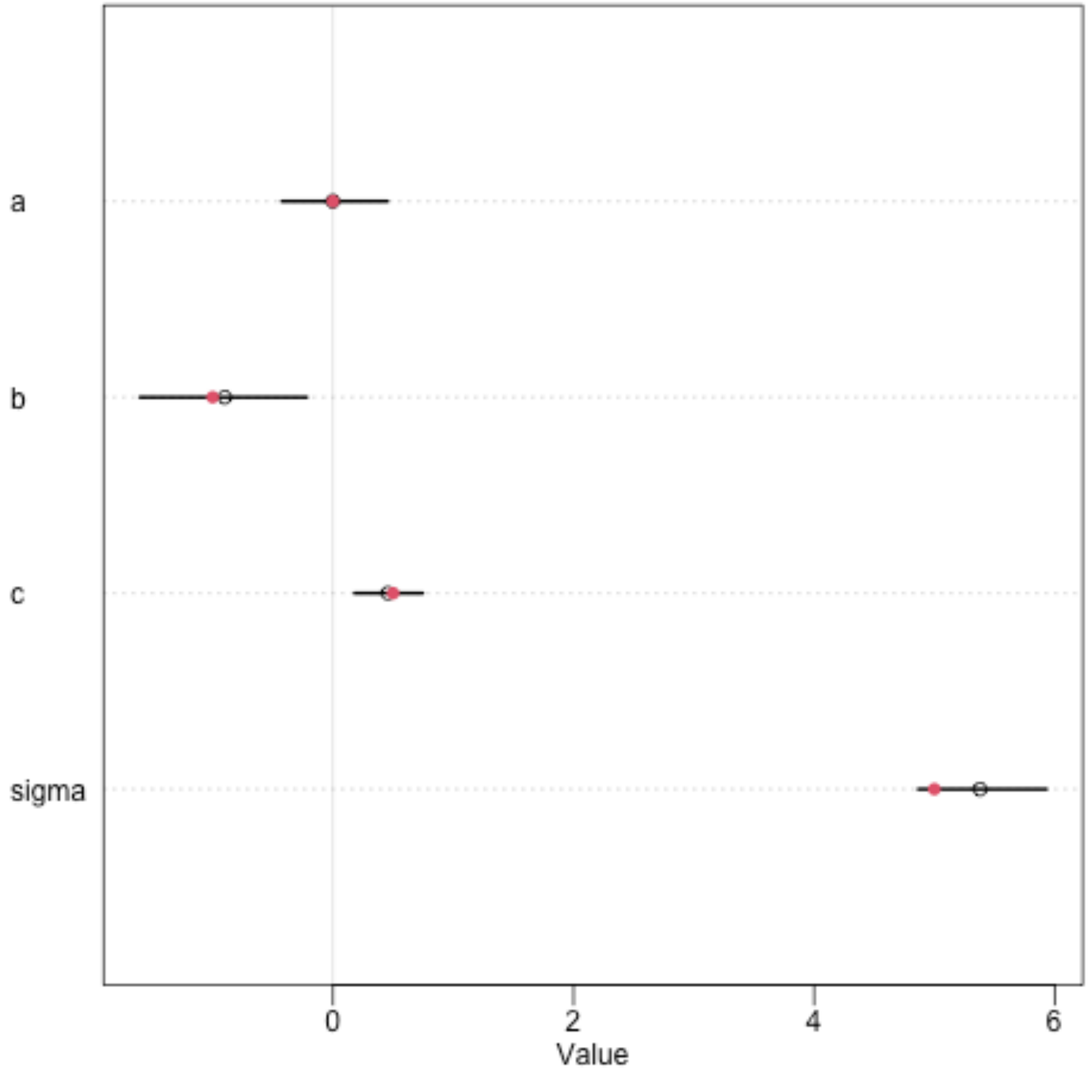
Simulation:

$$age_i = Uniform(0,\ 50)$$
$$toxin_i = Normal(10 + 0.4 \times age_i,\ 1)$$
$$size_i = Normal(30 - 1 \times toxin_i + 0.5 \times age_i,\ 5)$$

Model:

$$size_i \sim Normal(\mu_i, \sigma)$$
$$\mu_i = a + b \times toxin_i\ +\ c \times age$$

Exercise: What happens if we don't include age?



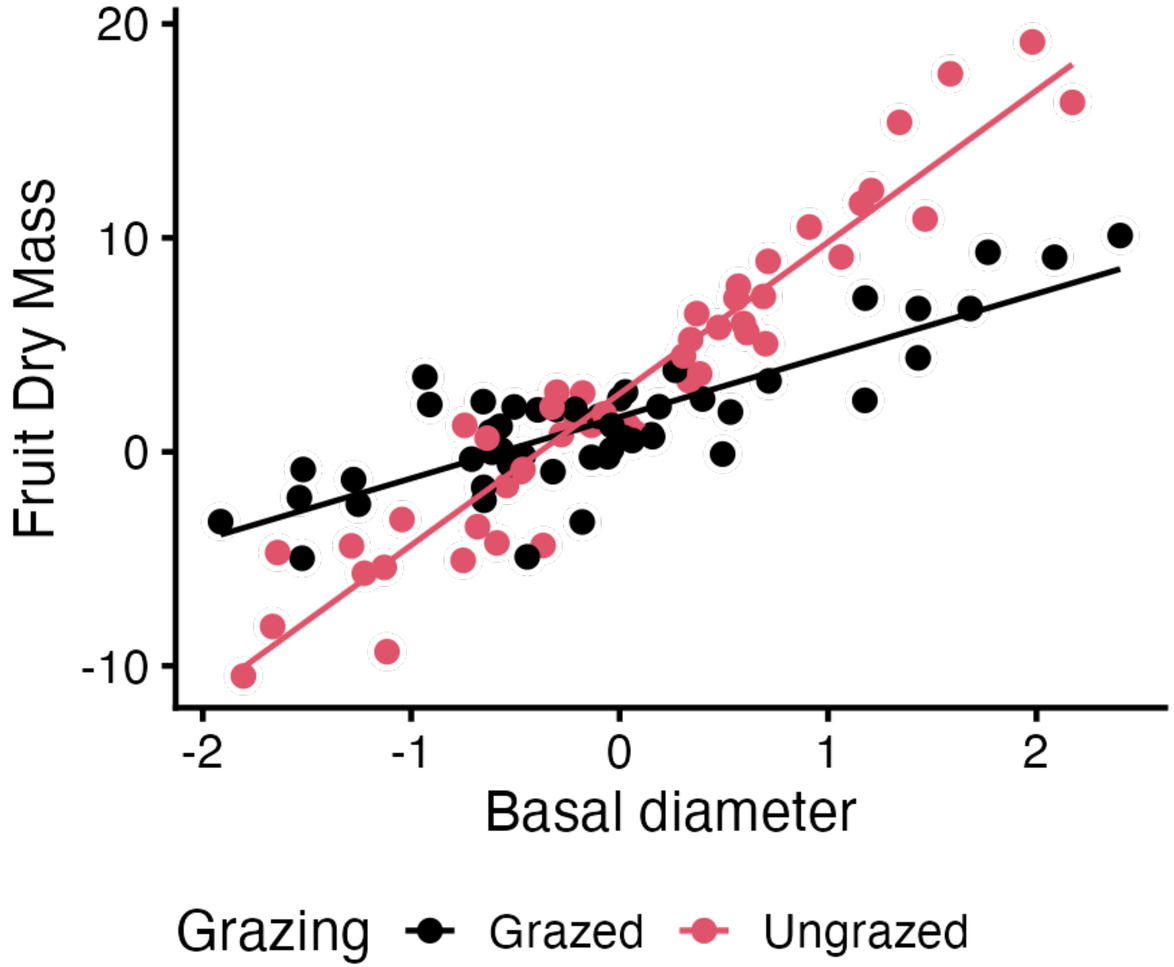
If your model doesn’t work on **simulated** data, it will **never** work on **real** data!

Interactions

Allowing coefficients to change according to other variables

- What if the relation between a predictor and an outcome changes depending on another predictor?
- We can account for this by adding product terms in the model
  - With two predictors, x and z:

$$\mu = \alpha + \beta_1 x + \beta_2 z + \beta_3 xz$$



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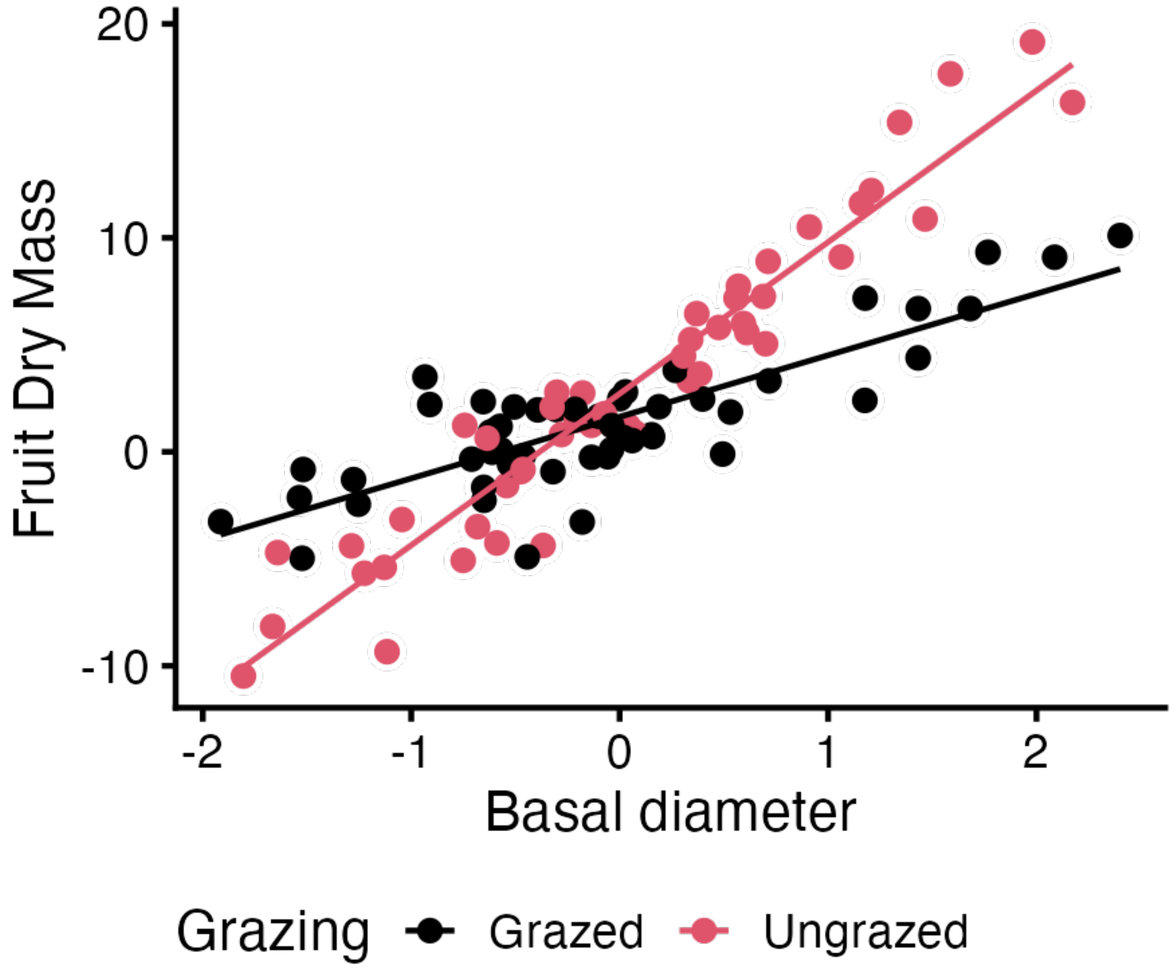
Interaction term!



Example with interactions

- **Question**: what are the best soil moisture and light availability to grow tulips?
- Greenhouse experiment: beds of tulips kept in nine combinations of soil moisture and shading. Three replicates for each combination (total of 27 beds).
- **Response variable**: mean plant height in each bed
- **Predictor variables**:
  - Water: 3 levels (low, med, high)
  - Shade: 3 levels (low, med, high)

Data from: Grafen & Hails (2002) Modern Statistics for the Life Sciences.

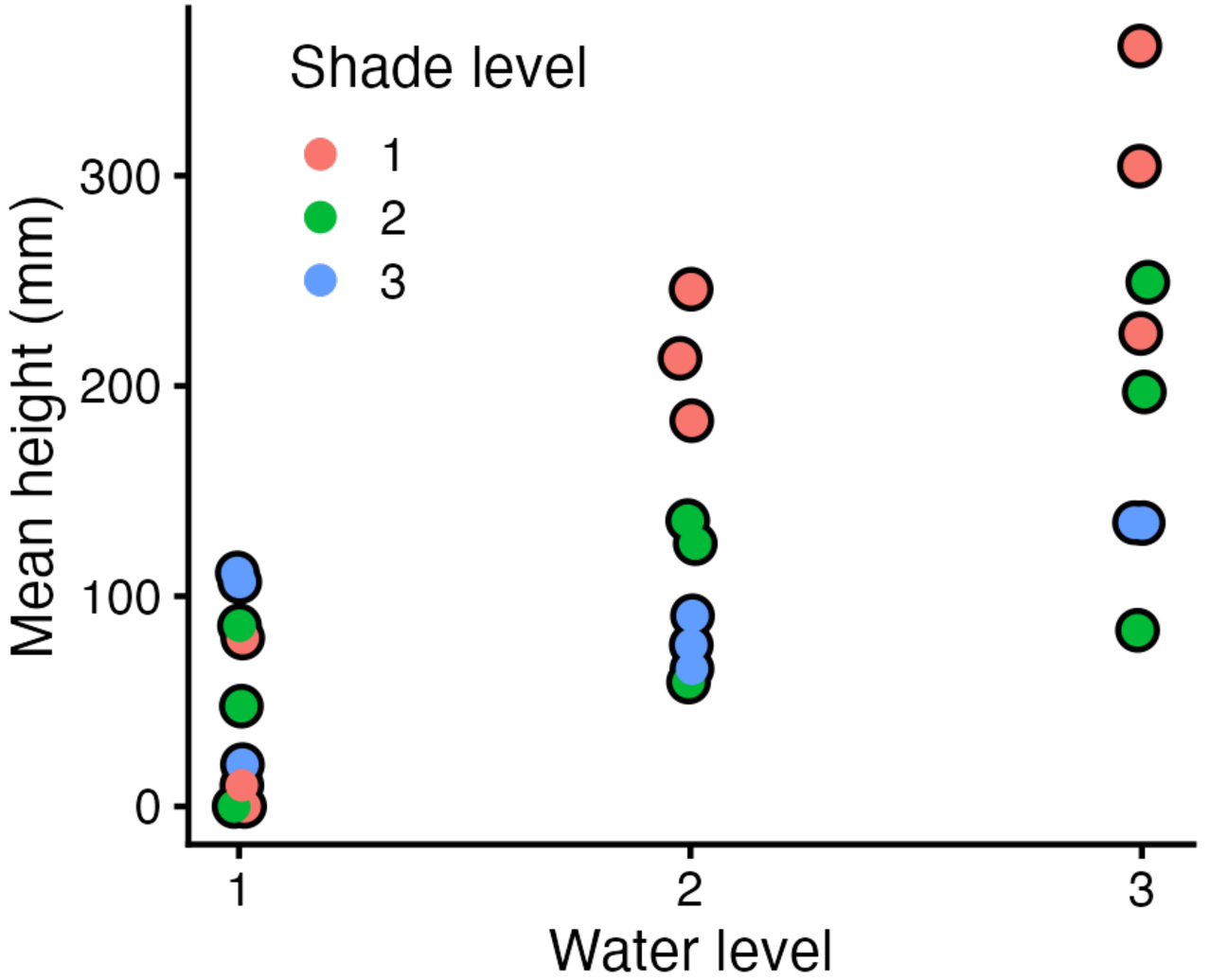
Tulips data

Shade level:

1. Low
2. Medium
3. High

Water level:

1. Low
2. Medium
3. High



Quick transformations

Always think about a scale that makes the model easier to interpret!

Shade level:

-1 : Low

0: Medium

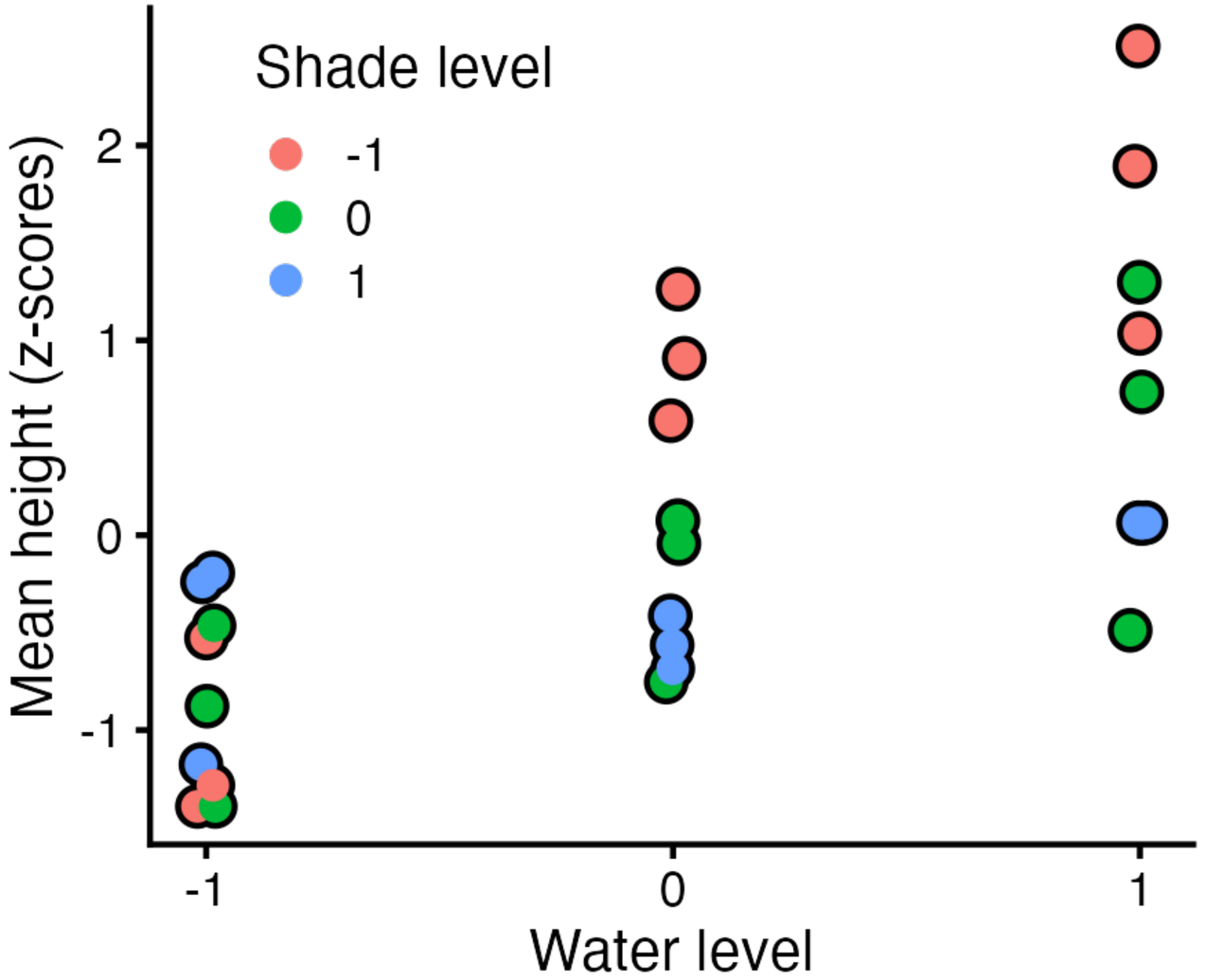
1: High

Water level:

-1 : Low

0: Medium

1: High

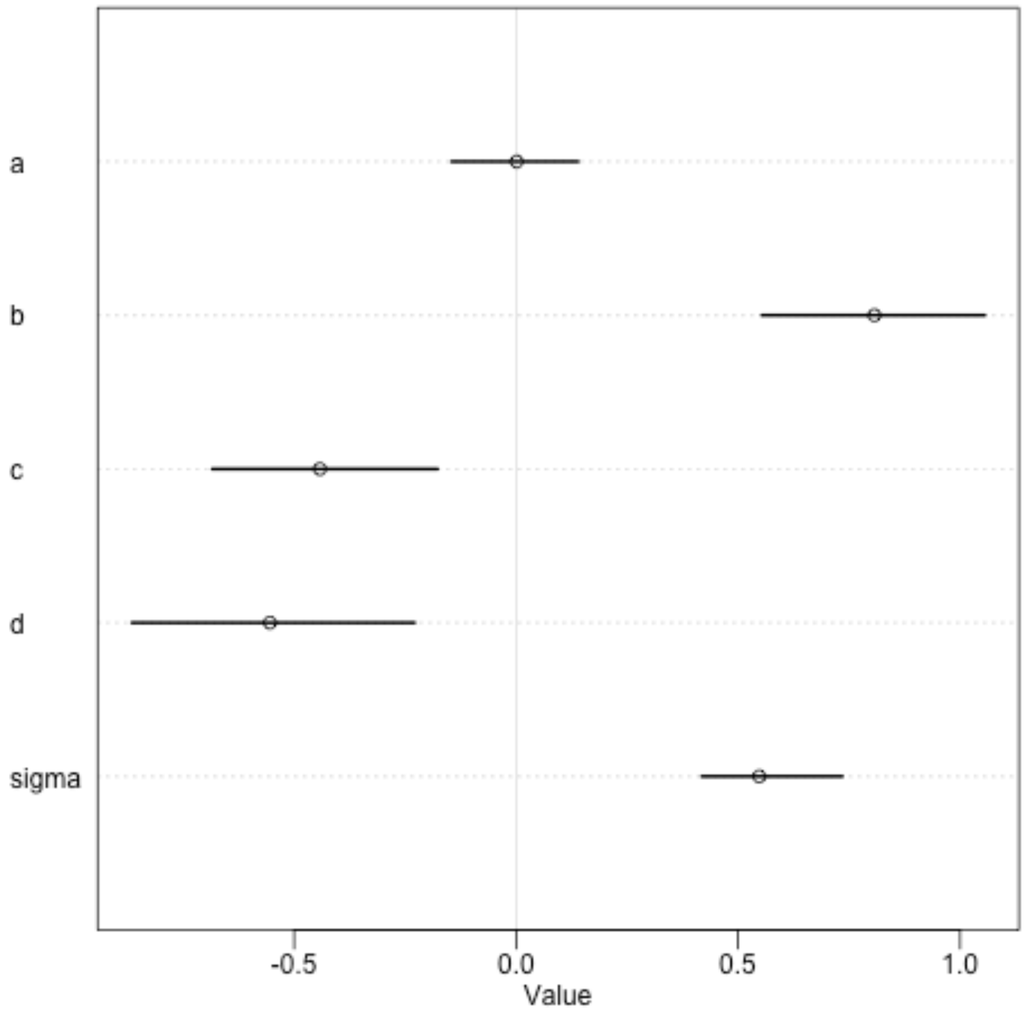


Model with interaction

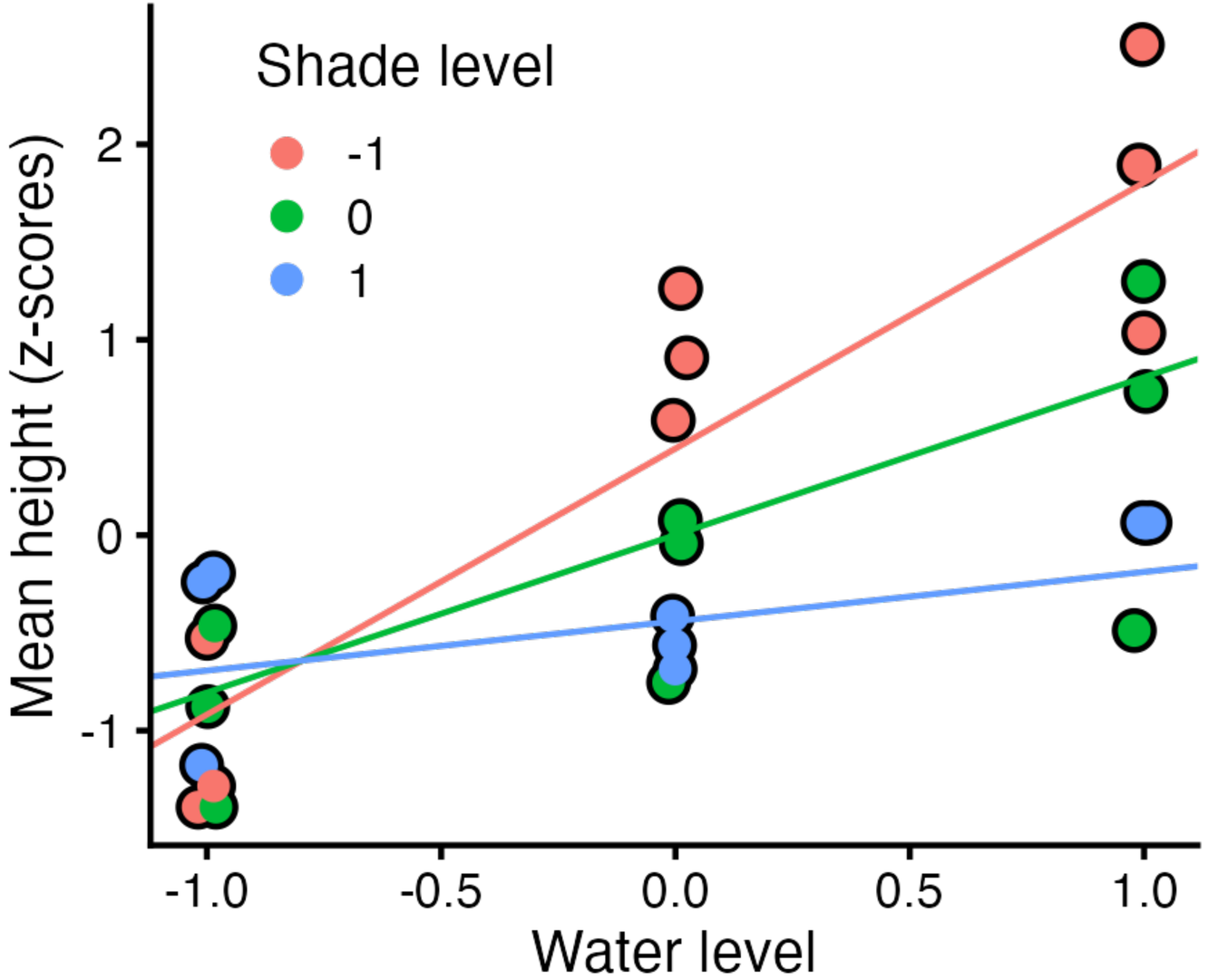
$$Height_i \sim Normal(\mu_i, \sigma)$$

$$\mu_i = a + b\ water_i + c\ shade + d\ water_i \times shade_i$$

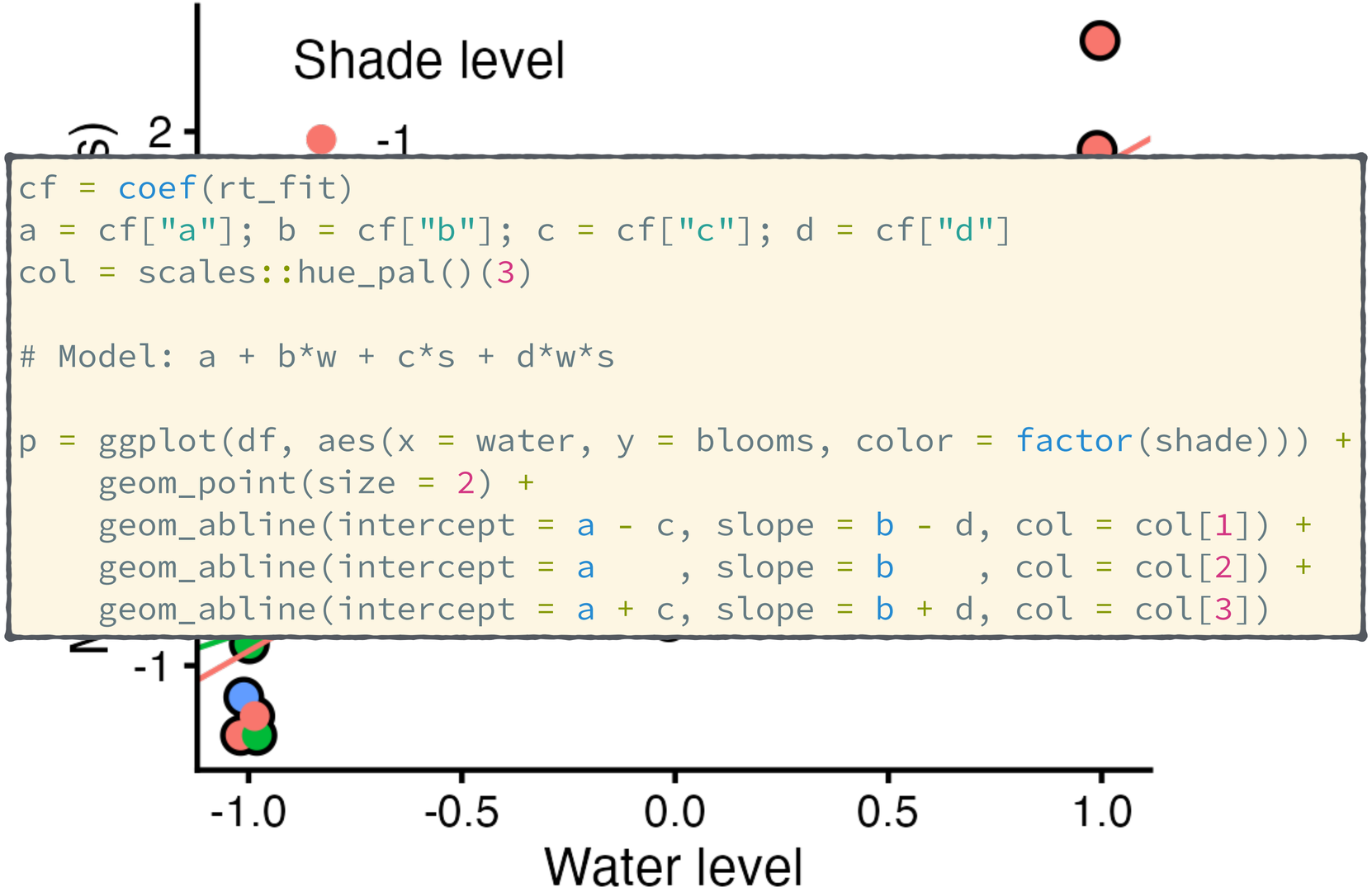
```
data("tulips")
df = tulips
df$water  = scale(df$water, scale = FALSE)
df$shade  = scale(df$shade, scale = FALSE)
df$blooms = scale(df$blooms)

rt_fit = ulam(alist(blooms ~ normal(mu, sigma),
            mu <- a + b*water + c*shade + d*water*shade,
            a ~ normal(0, 0.1),
            b ~ normal(0, 1),
            c ~ normal(0, 1),
            d ~ normal(0, 1),
            sigma ~ exponential(1)),
          data = df, chains = 4, cores = 4)
```



Prediction lines



Prediction lines




```r
cf = coef(rt_fit)
a = cf["a"]; b = cf["b"]; c = cf["c"]; d = cf["d"]
col = scales::hue_pal()(3)

# Model: a + b*w + c*s + d*w*s

p = ggplot(df, aes(x = water, y = blooms, color = factor(shade))) +
    geom_point(size = 2) +
    geom_abline(intercept = a - c, slope = b - d, col = col[1]) +
    geom_abline(intercept = a    , slope = b    , col = col[2]) +
    geom_abline(intercept = a + c, slope = b + d, col = col[3])
```

Summary

- Multiple linear models allow us to use more than one predictor in a linear model
- These models do a form of automatic **stratification**
  - **Ex:** difference in size for individuals of the same age, effect of treatment for individuals of the same size
- The objetive is to compare **like-to-like**

- Coefficients can and do change with the inclusion of more predictors
- Coefficient interpretation is hard, use plots, predictions, scaling and transformations to make models easier to interpret
- Next week, we talk about principled ways of choosing if a variable should be added to a model, stay tuned!