

Linear Models

Introduction to R - Day 3

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A little bit of theoretical background

Linear models background

The data:

- Random sample of n data points ($Y_i, X_{i1}, X_{i2}, \dots, X_{ip}, i = 1 \dots n$)
 - $X_{i1}, X_{i2}, \dots, X_{ip}$ are p independent predictor variables
 - Y_i is the dependent observation and response variable

The model:

$$Y_i = \beta_0 + \beta_1 * X_{1,i} + \beta_2 * X_{2,i} + \epsilon$$

- Y_i value of response variable
- $\beta_0, \beta_1, \beta_2$ model coefficients
- $X_{1,i}$ value of predictor X_1
- $X_{2,i}$ value of predictor X_2
- ϵ error term

Linear models background

$$Y_i = \beta_0 + \beta_1 * X_{1,i} + \beta_2 * X_{2,i} + \epsilon$$

Linear regression

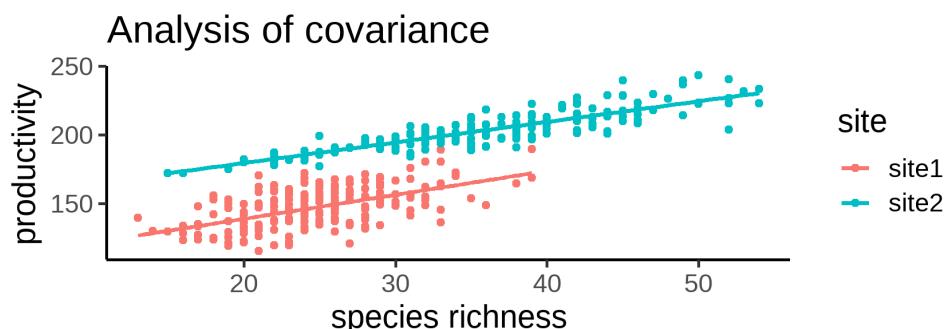
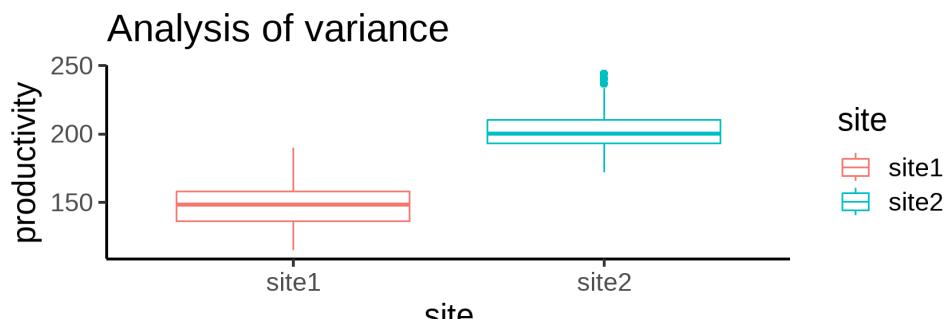
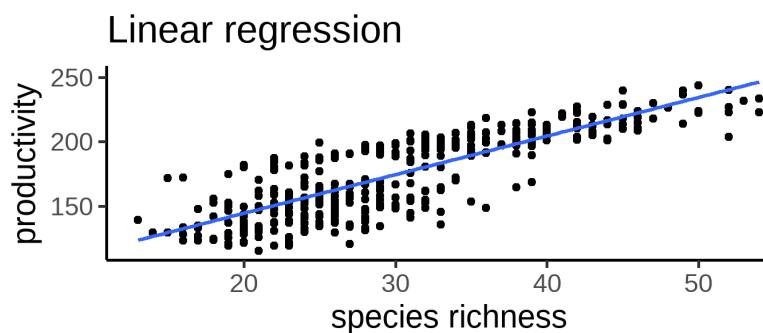
- numerical response
- numerical predictor(s)

Analysis of variance

- numerical response
- categorical predictor(s)

Analysis of covariance

- numerical response
- numerical and categorical predictor(s)



Goodness of fit linear model

Model residuals

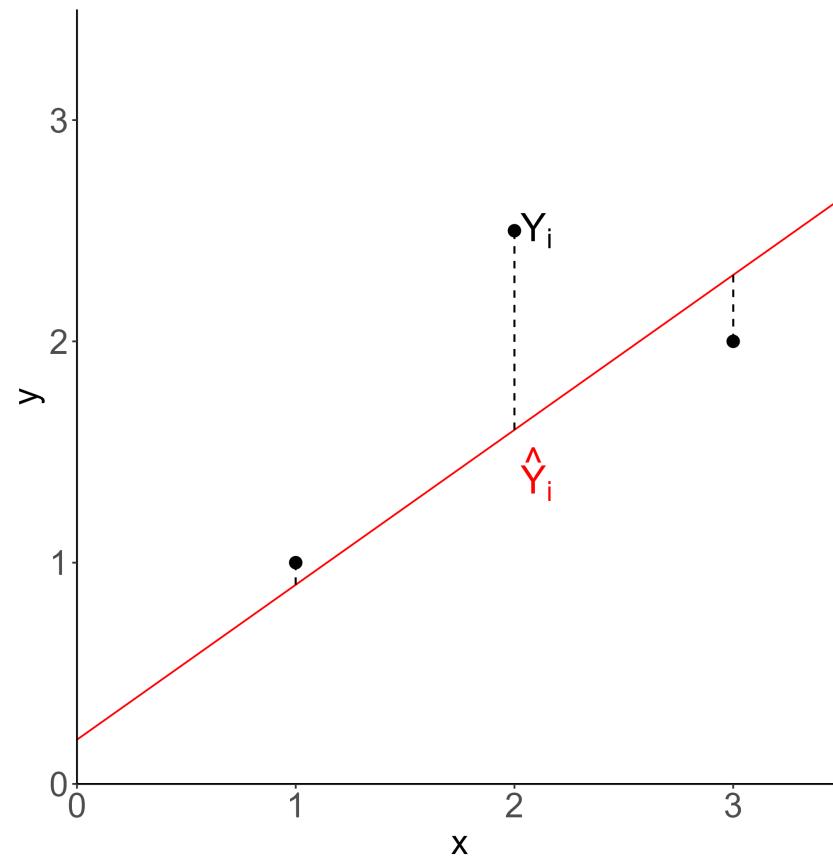
$$Y_i - \hat{Y}_i$$

Residual sum of squares (RSS)

$$RSS = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

Aim of the model fitting:

Find the model coefficients that lead to the lowest sum of squares.



Assumptions for linear models

Finding the model estimates that lead to the lowest residual sum of squares works only if:

- 1) Residuals are normally distributed
- 2) Residual variance is constant
- 3) No strong outliers

This has to be checked for every linear model!

If assumptions are not fulfilled, a different model approach has to be chosen.

How to fit linear models in

The data

We use productivity data from grassland sites.

The data set is called `prod` and has 3 variables: site, productivity and richness (species richness):

```
prod

## # A tibble: 400 × 3
##   site   richness productivity
##   <fct>    <dbl>        <dbl>
## 1 site1      23        122.
## 2 site1      26        158.
## 3 site1      24        165
## 4 site1      25        165.
## # ... with 396 more rows
```

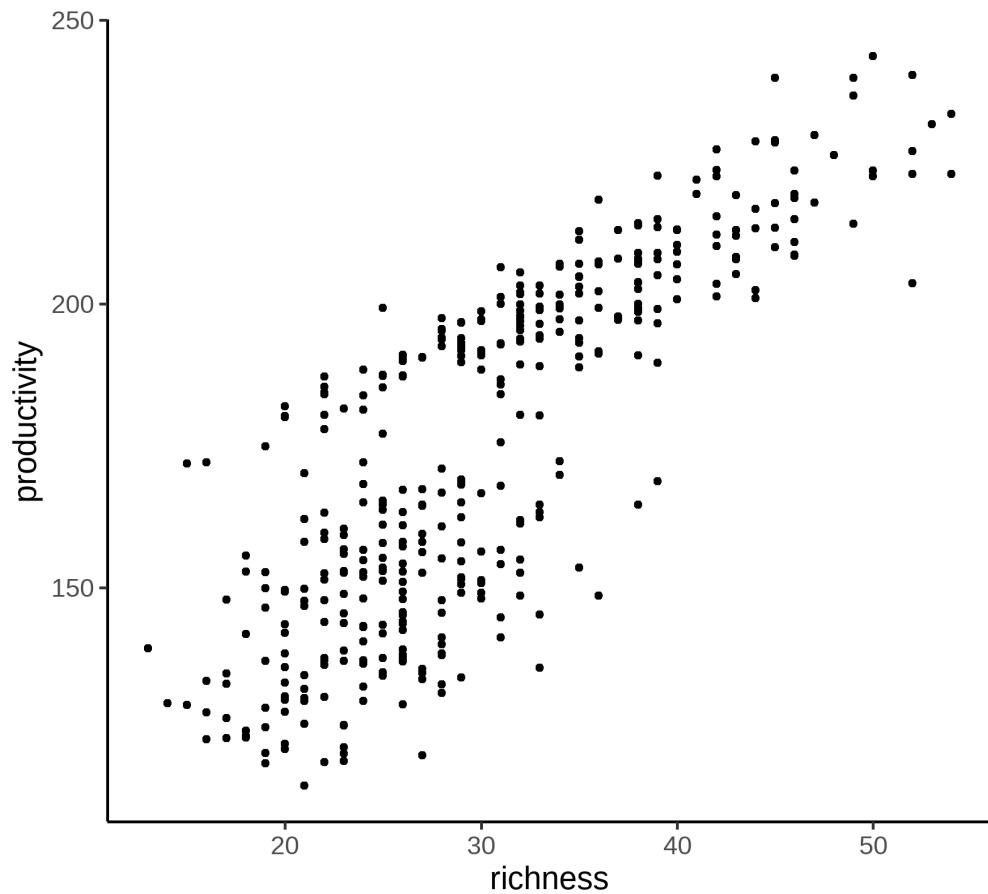
The variable site is a factor with two levels: site1 and site2

```
levels(prod$site) # get all levels of the factor
## [1] "site1" "site2"
```

Linear regression in

Linear regression in R

H_1 : Species richness has an effect on productivity



Linear regression in R

Use the `lm` function to fit a linear model in R.

The general structure of the function call is like this:

```
lm ( formula = Y ~ X, data = dat )
```

with

- `Y` being the response variable
- `X` being the predictor(s)
- `dat` being the name of the data

Multiple predictors can be added with `+` and `:` depending on interaction:

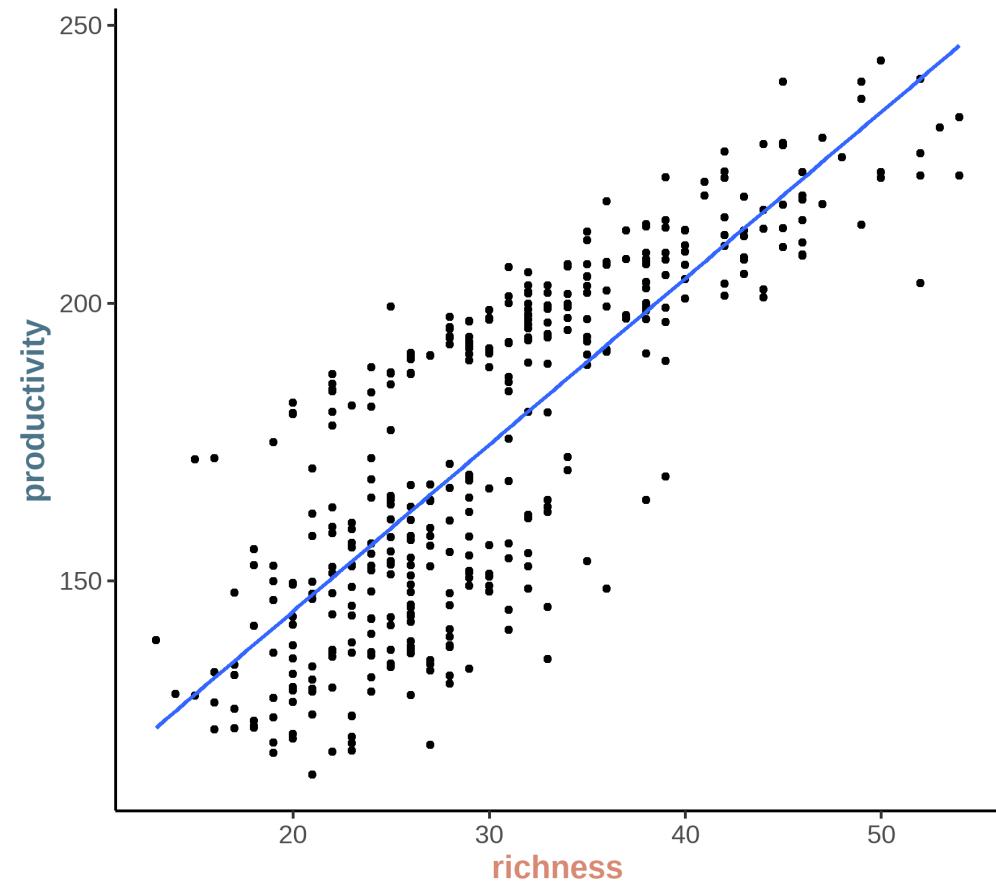
- `Y ~ x1 + x2` tests effects without interaction
- `Y ~ x1 + x2 + x1:x2` tests single effects and interaction between `x1` and `x2`

Linear regression in R

Let's fit a linear model to test our hypothesis

```
lm ( formula = Y ~ X, data = dat )
```

```
prod_lm <- lm(productivity ~ richness,  
                 data = prod)
```



Linear regression in R

Is the effect of richness on productivity significant?

Or in other words

Does the model with richness as predictor significantly reduce the residual sum of squares?

Hypothesis testing using F-Tests

Compare the complex model with a simple model that does not contain the predictor

H_0 : The error variance in the simple model is not significantly higher than in the more complex model

- H_0 accepted: simplification was justified → use simple model without predictor
- H_0 rejected: simplification reduced explanatory power → use complex model with predictor

Linear regression in R

Hypothesis testing using F-Tests in R

H_0 : The error variance in the simple model is not significantly higher than in the more complex model

`drop1` deletes single terms from the model and performs an F-test:

```
drop1(prod_lm, test = "F")
## Single term deletions
##
## Model:
## productivity ~ richness
##           Df Sum of Sq    RSS    AIC F value    Pr(>F)
## <none>          132779 2326.0
## richness  1     254119 386899 2751.8   761.71 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Result: Reject $H_0 \rightarrow$ Richness increases productivity ($F_{1,398} = 761.71, p < 0.001$)

Extracting the coefficients

Look at model coefficients using the model `summary`

```
summary(prod_lm)
##
## Call:
## lm(formula = productivity ~ richness, data = prod)
##
## Residuals:
##     Min      1Q  Median      3Q     Max 
## -47.593 -13.683   0.029  13.970  42.295 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 84.6982    3.3987  24.92   <2e-16 ***
## richness    2.9938    0.1085  27.60   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18.27 on 398 degrees of freedom
## Multiple R-squared:  0.6568,    Adjusted R-squared:  0.6559 
## F-statistic: 761.7 on 1 and 398 DF,  p-value: < 2.2e-16
```

Summary table

```
summary(prod_lm)
##
## Call:
## lm(formula = productivity ~ richness, data = prod)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -47.593 -13.683   0.029  13.970  42.295
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 84.6982    3.3987  24.92 <2e-16 ***
## richness    2.9938    0.1085  27.60 <2e-16 ***
## ---
## Signif. codes:  0 '****' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18.27 on 398 degrees of freedom
## Multiple R-squared:  0.6568,   Adjusted R-squared:  0.6559
## F-statistic: 761.7 on 1 and 398 DF,  p-value: < 2.2e-16
```

Calculated model

Distribution of residuals (errors)

Summary table

```
summary(prod_lm)
##
## Call:
## lm(formula = productivity ~ richness, data = prod)
## Model coefficients:
## 1. Intercept = 84.7
## 2. Slope = 3
## -47.593 -13.683   Median 0.029 18.970   Max 42.295
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 84.6982  3.3987  24.92 <2e-16 ***
## richness    2.9938  0.1085  27.60 <2e-16 ***
## ---
## Signif. codes:  0 '****' 0.001 '***' 0.01 '**' 0.05 '*' 0.1 '.' 1
##
## Residual standard error: 18.27 on 398 degrees of freedom
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Summary table

```
summary(prod_lm)
##
## Call:
## lm(formula = productivity ~ richness, data = prod)
##
## Residuals:
##     Min      1Q  Median      3Q     Max 
## -47.593 -13.683   0.029  13.970  42.295 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 84.6982    3.3987  24.92   <2e-16 ***
## richness    2.9938    0.1085  27.60   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18.27 on 398 degrees of freedom
## Multiple R-squared:  0.6568, Adjusted R-squared:  0.6559 
## F-statistic: 761.7 on 1 and 398 DF, p-value: < 2.2e-16
```

t-statistics: ratio of coefficients to their standard error

Summary table

```
summary(prod_lm)
##
## Call:
## lm(formula = productivity ~ richness, data = prod)
##
## Residuals:
##     Min      1Q  Median      3Q     Max 
## -47.593 -13.683   0.029  13.970  42.295 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 84.6982    3.3987  24.92   <2e-16 ***
## richness    2.9938    0.1085  27.60   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.01 '**' 0.05 '*' 0.1 '.' 1
## 
## Coefficient of determination R2
## 
## Residual standard error: 18.27 on 398 degrees of freedom
## Multiple R-squared:  0.6568, Adjusted R-squared:  0.6559 
## F-statistic: 761.7 on 1 and 398 DF, p-value: < 2.2e-16
```

Test model assumptions

Test model assumptions to make sure that:

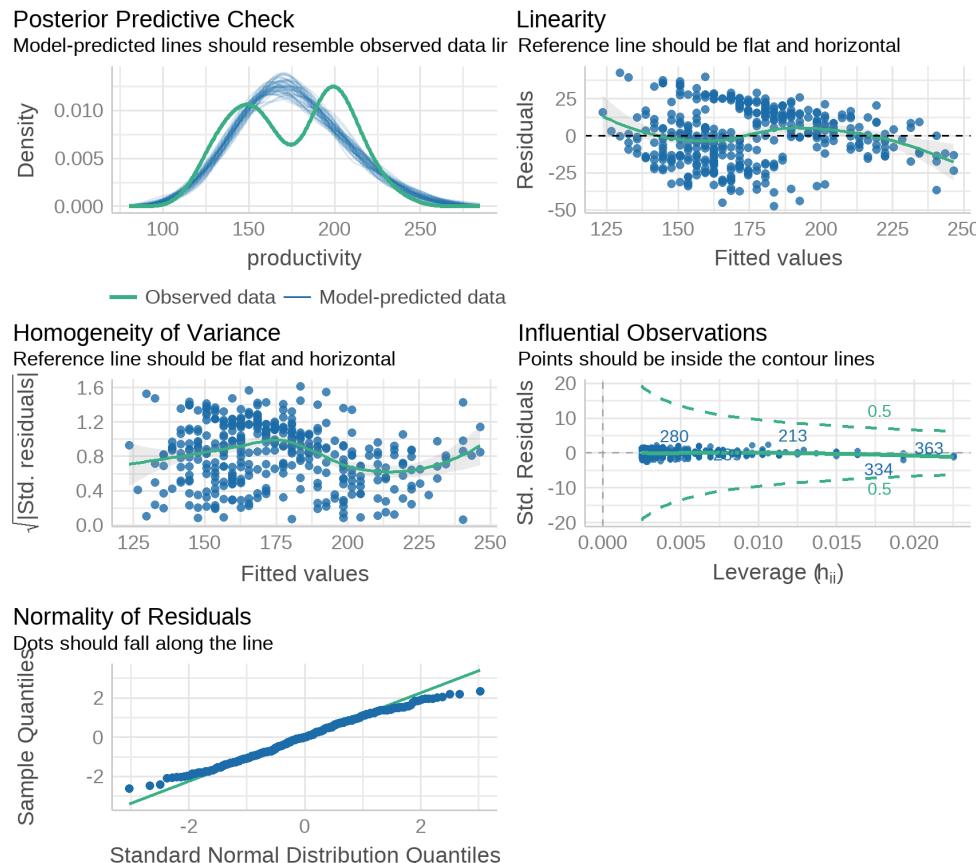
- 1) Residuals are normally distributed
- 2) Variance is constant (homogeneous)
- 3) There are no strong outliers or very influential observations

We can check that by looking at diagnostic plots

```
# install.packages("performance")
performance::check_model(prod_lm)
```

Test model assumptions

```
performance::check_model(prod_lm)
```



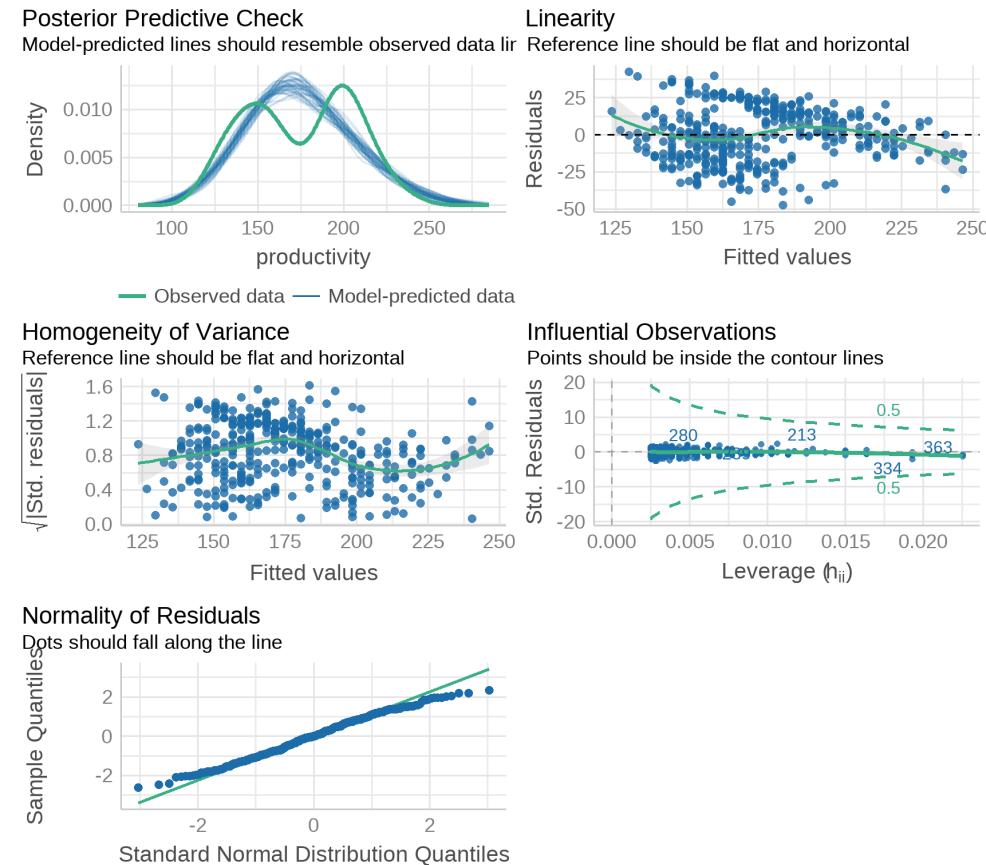
Test model assumptions

Check the assumptions

- Residuals are normally distributed ✓
- Variance is constant (homogeneous) ✓
- There are no strong outliers or very influential observations ✓

Checking diagnostic plots needs some experience

- Real life data (almost) never perfectly fit the assumptions
- Linear models are to some extent robust against violations of the assumptions



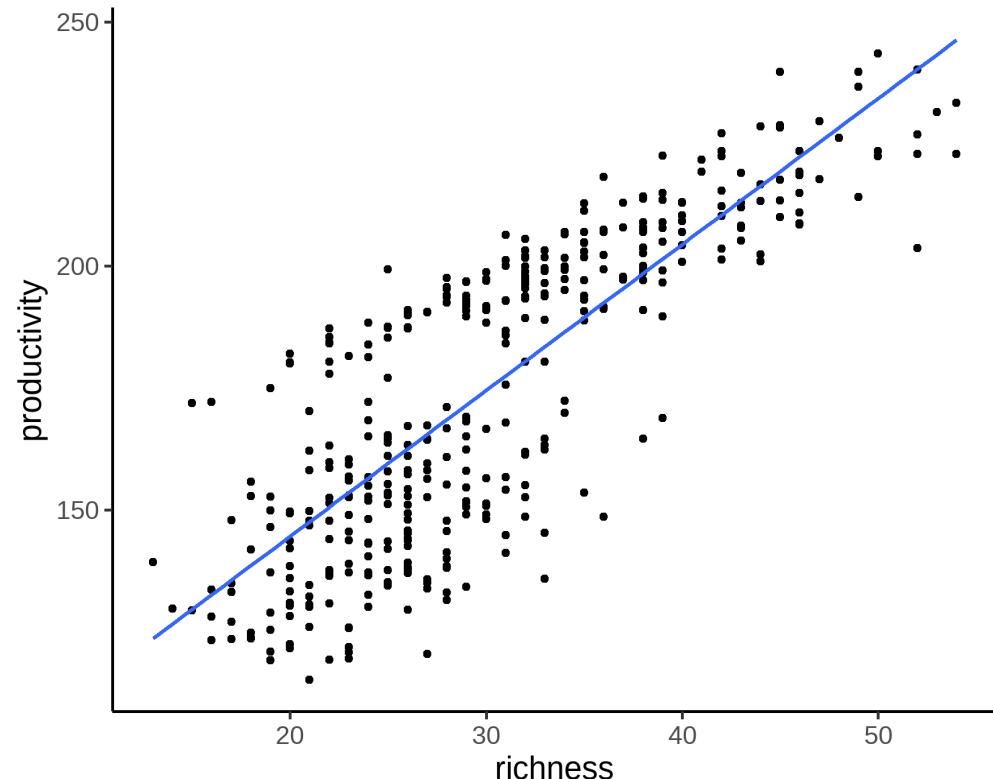
Plot the model

Option 1

Add the regression line directly as a ggplot layer

Use `geom_smooth()` to add the model directly:

```
ggplot(prod, aes(x = richness, y =  
productivity)) +  
  geom_point() +  
  geom_smooth(method = "lm", se = FALSE)
```



Plot the model

Option 2

Extract coefficients (slope + intercept) of the model and add the regression line

```
# These are the coefficients of the lm  
prod_lm$coefficients  
## (Intercept)    richness  
##     84.698163    2.993774
```

```
intercept <- prod_lm$coefficients[1]  
slope <- prod_lm$coefficients[2]
```

Plot the model

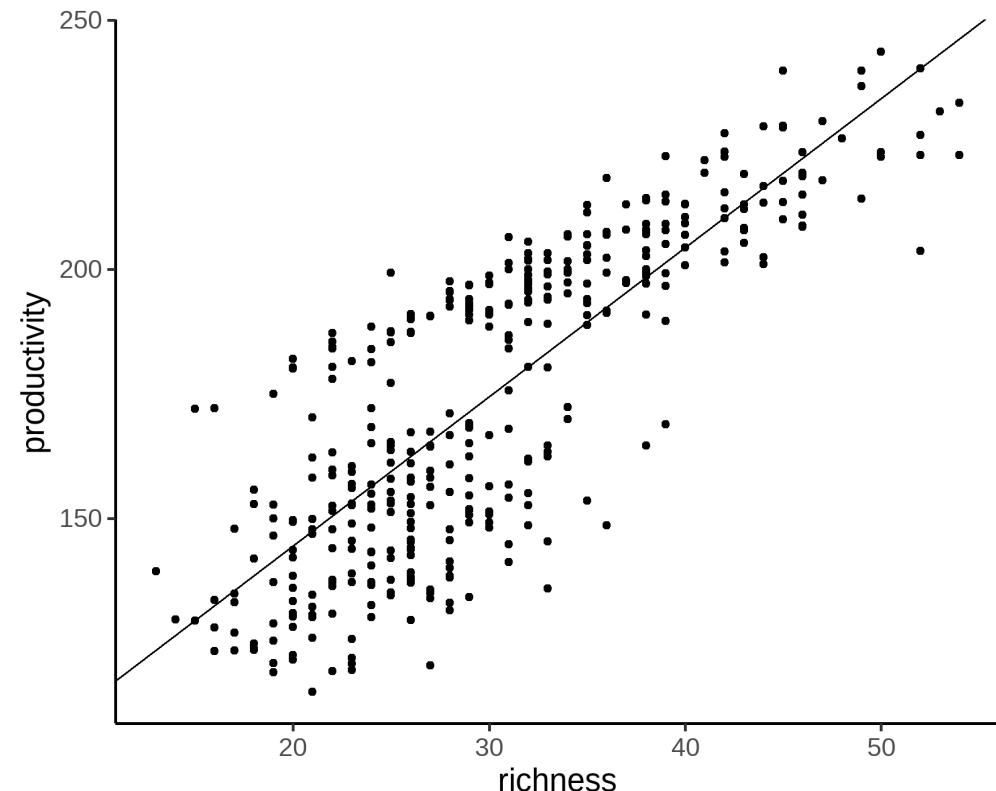
Option 2

Extract coefficients (slope + intercept) of the model and add the regression line

```
intercept <- prod_lm$coefficients[1]  
slope <- prod_lm$coefficients[2]
```

Add a line defined by slope and intercept using
`geom_abline()`:

```
ggplot(prod, aes(x=richness, y=productivity)) +  
  geom_point() +  
  geom_abline(slope = slope,  
             intercept = intercept)
```

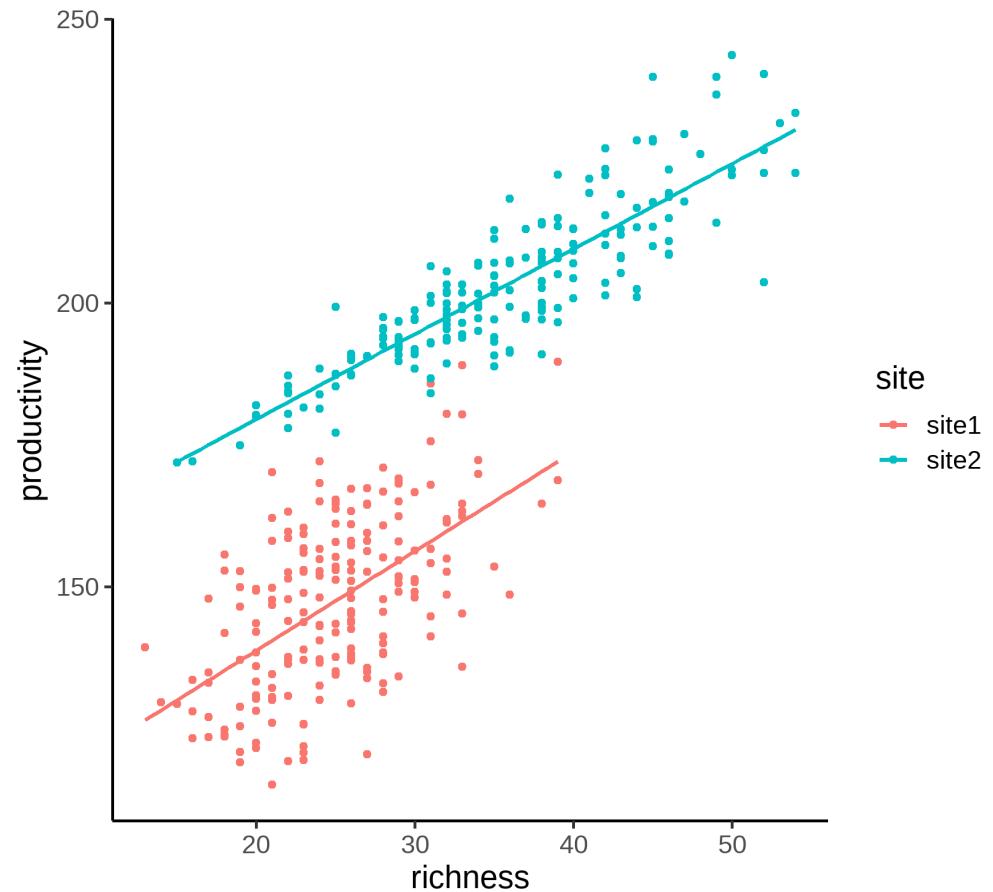
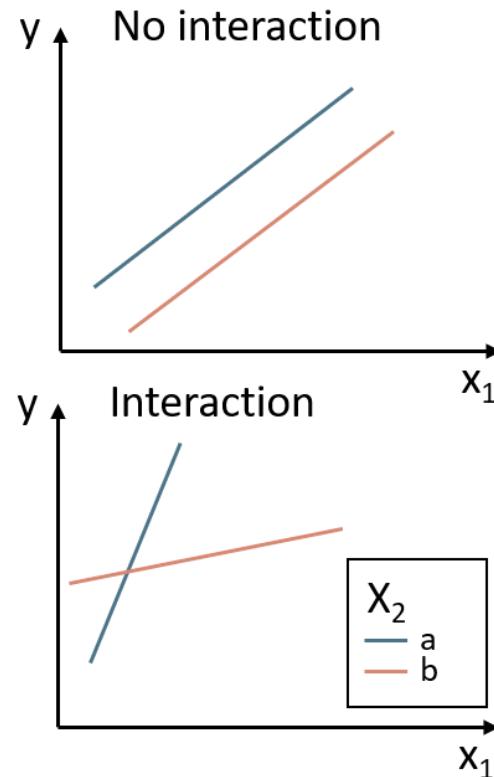


Analysis of covariance

Analysis of covariance

One categorical and one numerical predictor variable

Two possible models:



Linear models background

Linear relation with two predictors X_1 and X_2 ($i = 1 \dots n$)

Without interaction

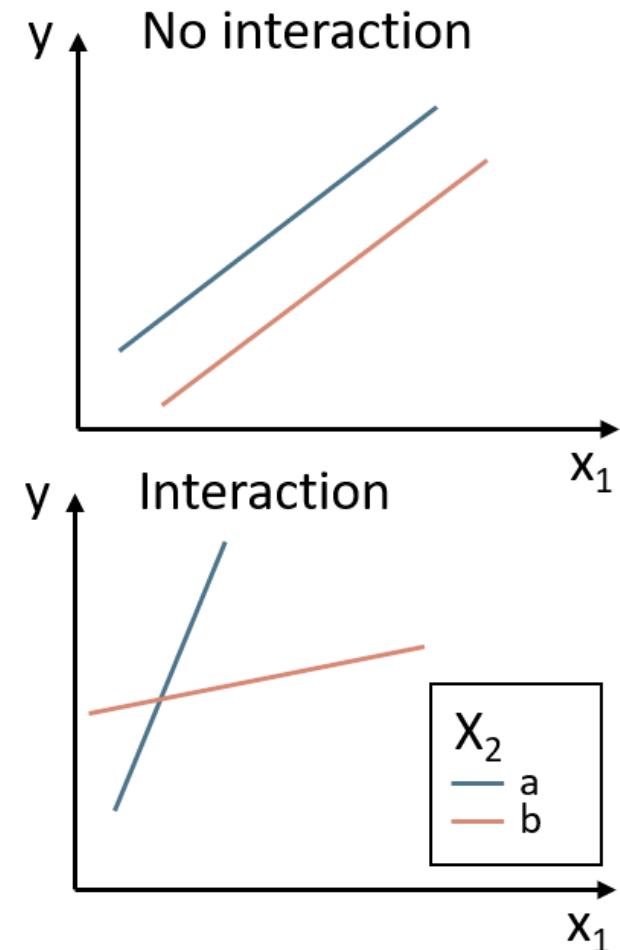
$$Y_i = \beta_0 + \beta_1 * X_{1,i} + \beta_2 * X_{2,i} + \epsilon$$

With interaction

$$Y_i = \beta_0 + \beta_1 * X_{1,i} + \beta_2 * X_{2,i} + \beta_3 * X_{1,i} * X_{2,i} + \epsilon$$

with

- Y_i value of response variable
- $\beta_0, \beta_1, \beta_2$ model coefficients
- $X_{1,i}$ value of predictor X_1
- $X_{2,i}$ value of predictor X_2
- ϵ error term



Analysis of covariance

Fit the model with `lm`

Without interaction

Species richness has an effect on productivity and there is a difference between sites.

```
prod_lm2a <- lm(productivity ~ richness + site, data = prod)
```

With interaction

Species richness has an effect on productivity and the effect differs between sites.

```
prod_lm2b <- lm(productivity ~ richness + site + richness:site, data = prod)
```

Analysis of covariance

Are the effects significant?

Without interaction

```
drop1(prod_lm2a, test = "F") # no interaction
## Single term deletions
##
## Model:
## productivity ~ richness + site
##           Df Sum of Sq    RSS    AIC F value    Pr(>F)
## <none>            40064 1848.7
## richness   1     42908  82973 2137.9  425.18 < 2.2e-16 ***
## site       1     92715 132779 2326.0  918.72 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Both, the removal of site and richness significantly increase the model's RSS → both site and richness are significant predictors

Analysis of covariance

Are the effects significant?

With interaction

```
drop1(prod_lm2b, test = "F") # interaction
## Single term deletions
##
## Model:
## productivity ~ richness + site + richness:site
##           Df Sum of Sq   RSS   AIC F value Pr(>F)
## <none>            39850 1848.6
## richness:site     1    214.53 40064 1848.7  2.1319 0.1451
```

The removal of the interaction does not significantly increase the model's RSS → the interaction is not significant and the simpler model without interaction is just as good in predicting productivity.

Extracting model coefficients

```
summary(prod_lm2a)
##
## Call:
## lm(formula = productivity ~ richness + site, data = prod)
##
## Residuals:
##       Min     1Q Median     3Q    Max
## -30.1743 -6.2895 -0.0352  5.6955 28.9276
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 108.36550   2.02582  53.49 <2e-16 ***
## richness     1.56699   0.07599  20.62 <2e-16 ***
## sitesite2    38.78575   1.27962  30.31 <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 10.05 on 397 degrees of freedom
## Multiple R-squared:  0.8964,    Adjusted R-squared:  0.8959 
## F-statistic: 1718 on 2 and 397 DF,  p-value: < 2.2e-16
```

Extracting model coefficients

Call:

```
lm(formula = productivity ~ richness + site, data = prod)
```

Residuals:

Min	1Q	Median
-30.1743	-6.2895	-0.0352

Intercept site1 = 108.4

Slope = 1.6

Intercept site2 = 108.4 + 38.8

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	108.36550	2.02582	53.49	<2e-16	***
richness	1.56699	0.07599	20.62	<2e-16	***
sitesite2	38.78575	1.27962	30.31	<2e-16	***

Signif. codes: 0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 10.05 on 397 degrees of freedom

Multiple R-squared: 0.8964, Adjusted R-squared: 0.8959

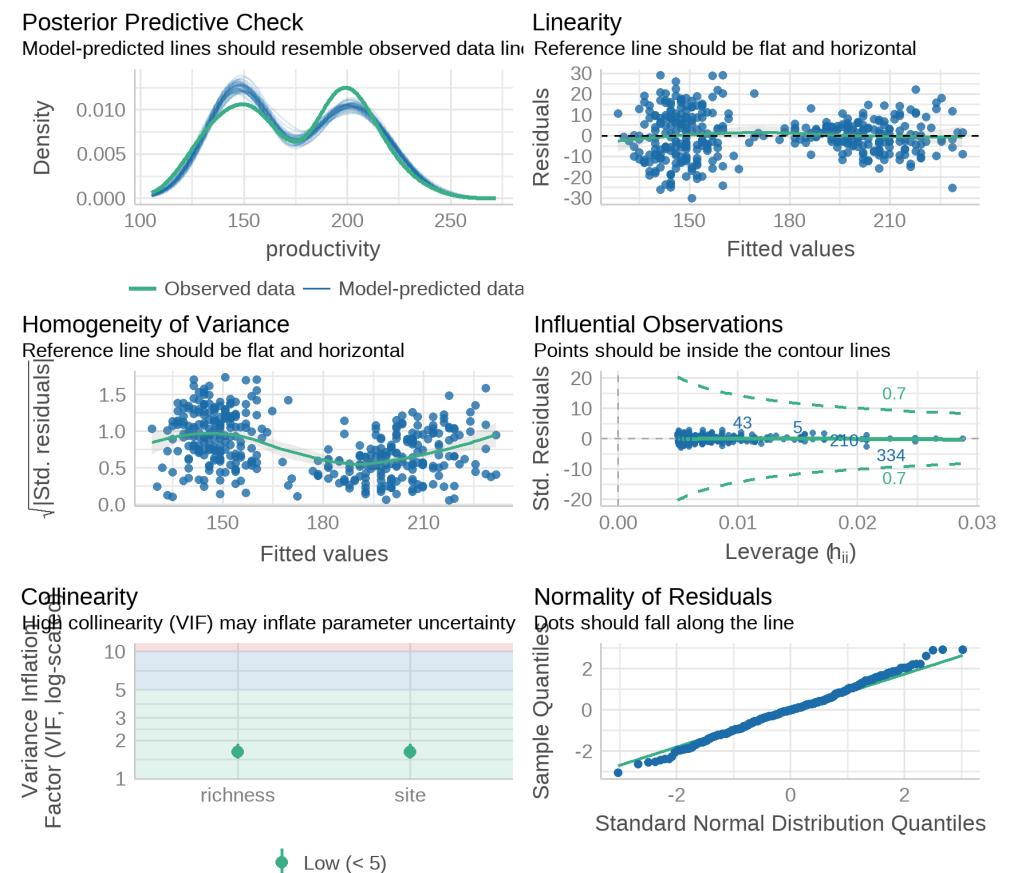
F-statistic: 1718 on 2 and 397 DF, p-value: < 2.2e-16

Test model assumptions

Check the assumptions

- Residuals are normally distributed ✓
- Variance is constant (homogeneous) ✓
- There are no strong outliers or very influential observations ✓

```
performance::check_model(prod_lm2a)
```

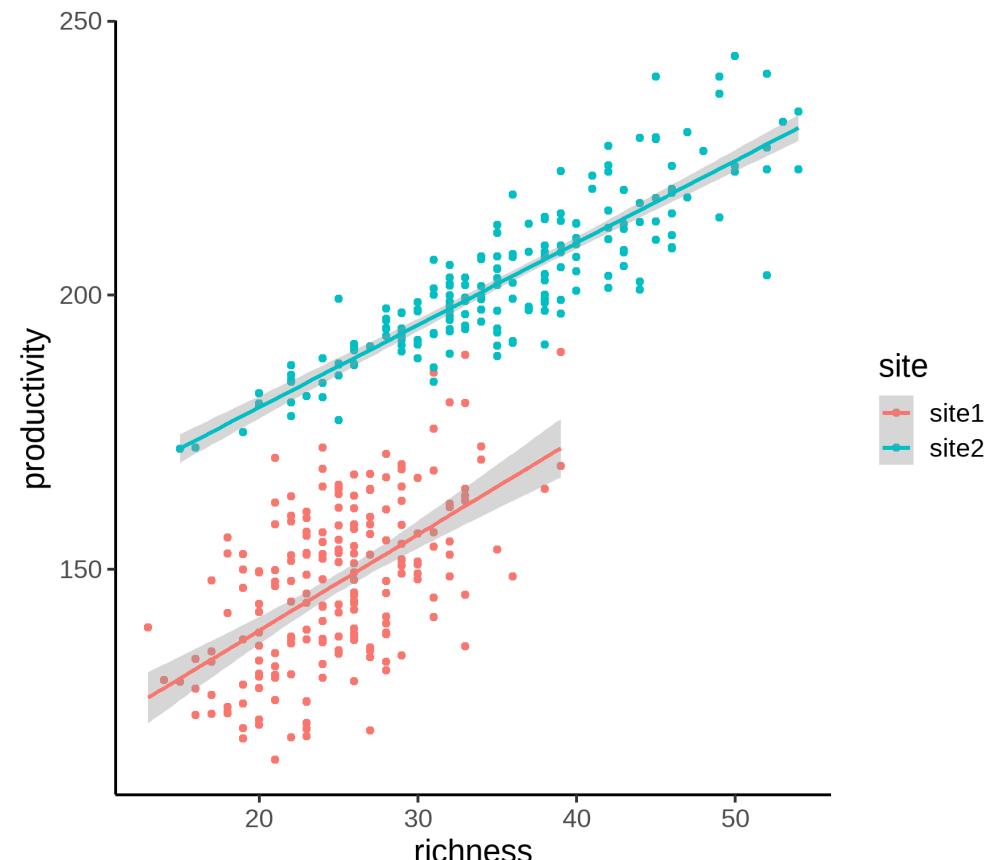


Plot the model

If we want to be precise, we could not use `geom_smooth()` for this model because it plots the full model with interaction between the predictors

```
ggplot(prod, aes(x = richness,
                  y = productivity,
                  color = site)) +
  geom_point() +
  geom_smooth(method = "lm")
```

This plot is not 100% appropriate if the model you present is without interaction



Plot the model

Extract coefficients and add regression line

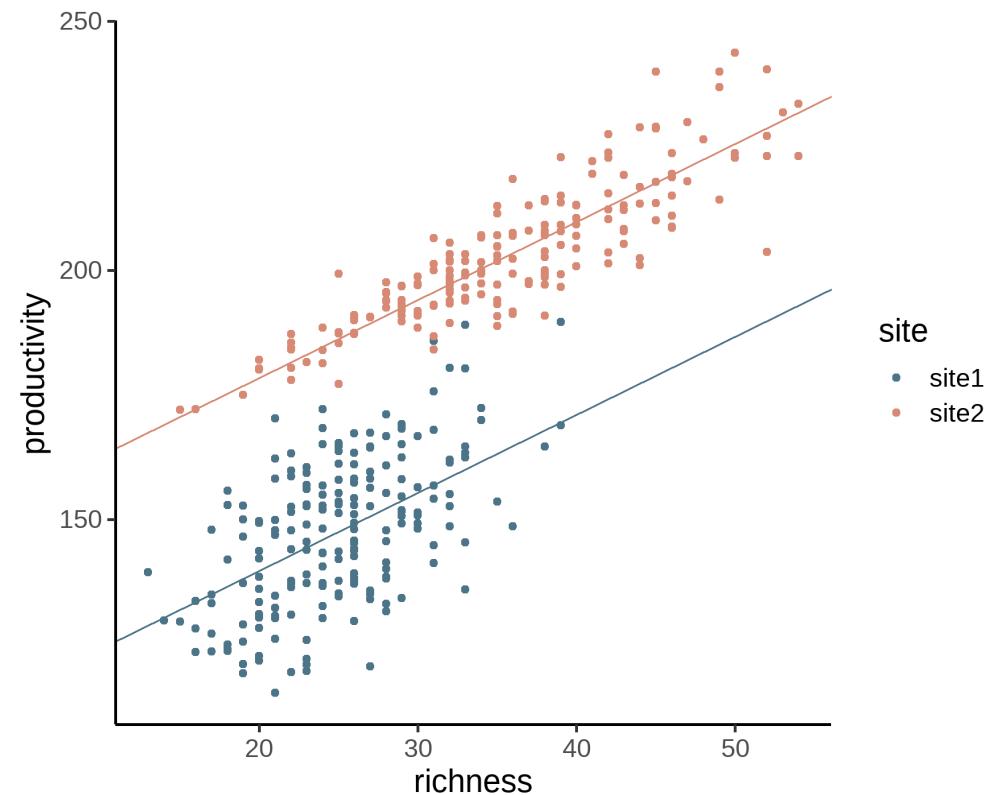
```
# these are the model coefficients
prod_lm2a$coefficients
## (Intercept)    richness   sitesite2
## 108.365497     1.566994   38.785753
```

```
slope <- prod_lm2a$coefficients[2]
intercept1 <- prod_lm2a$coefficients[1]
intercept2 <- prod_lm2a$coefficients[1] + prod_lm2a$coefficients[3]
```

Plot the model

Extract coefficients and add regression line

```
ggplot(prod, aes(x = richness,
                  y = productivity,
                  color = site)) +
  geom_point() +
  scale_color_manual(
    values = c("#4C7488", "#D78974")) +
  geom_abline(
    slope = slope,
    intercept = intercept1,
    color = "#4C7488"
  ) +
  geom_abline(
    slope = slope,
    intercept = intercept2,
    color = "#D78974"
  )
```



Plot the model

Option 2: Use the `predict()` function

```
# step 1: create some data to predict from
pred_data <- tidyverse::expand_grid(
  richness = min(prod$richness) : max(prod$richness),
  site = c("site1", "site2")
)
```

```
## # A tibble: 84 × 2
##   richness site
##       <int> <chr>
## 1        13 site1
## 2        13 site2
## 3        14 site1
## # ... with 81 more rows
```

- `tidyverse::expand_grid` returns a tibble with all combinations of site and richness given as input
 - The `tidyverse` package is part of the tidyverse
- The column names of the tibble that you create in this step have to correspond to the predictor names in the linear model

Plot the model

Option 2: Use the `predict()` function

```
# step 1: create some data to predict from
pred_data <- tidyverse::expand_grid(
  richness = min(prod$richness) : max(prod$richness),
  site = c("site1", "site2")
)
```

```
# step2: predict productivity values from pred_data
predictions <- predict(prod_lm2a, newdata = pred_data)
```

- `predict` uses the `prod_lm2a` model and the data produced with `expand_grid` to predict productivity values for each combination of site and richness.

Plot the model

Option 2: Use the `predict()` function

```
# step 1: create some data to predict from
pred_data <- tidyverse::expand_grid(
  richness = min(prod$richness) : max(prod$richness),
  site = c("site1", "site2")
)
```

```
# step 2: predict productivity values from pred_data
predictions <- predict(prod_lm2a, newdata = pred_data)
```

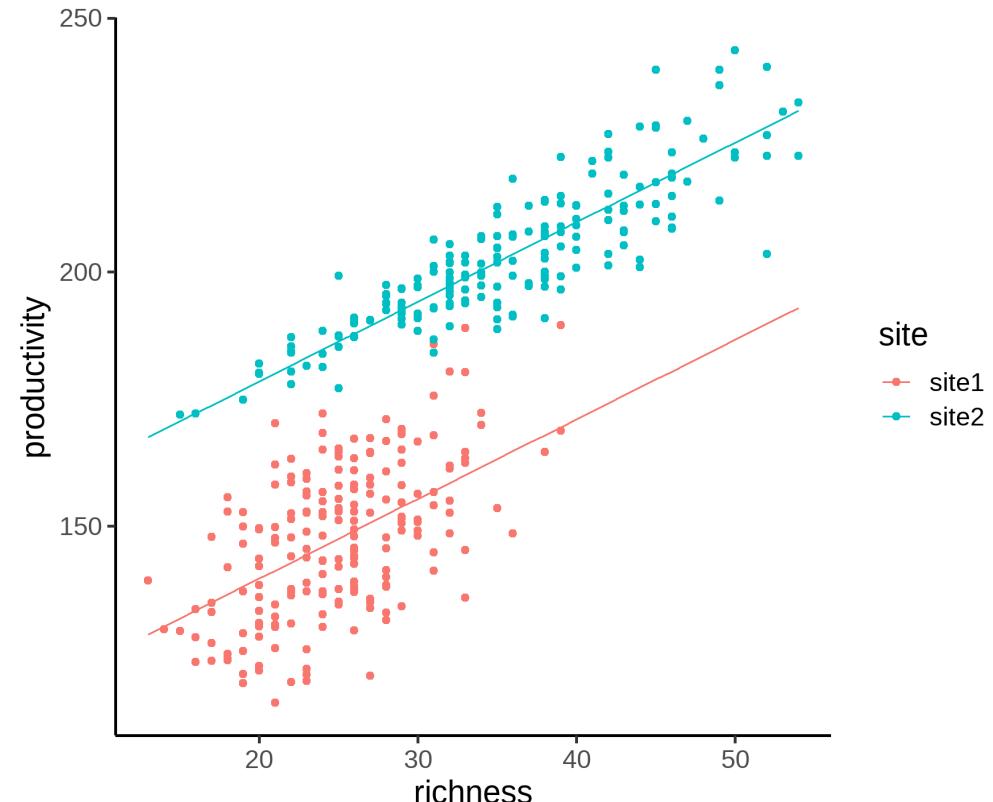
```
# step 3: add predictions to the tibble
pred_data$productivity <- predictions
```

Plot the model

Option 2: Use the `predict()` function

Add a new `geom_*` layer to the plot from the prediction data:

```
# step 4: Add predictions with geom_line
ggplot(prod, aes(x = richness,
                  y = productivity,
                  color = site)) +
  geom_point() +
  geom_line(data = pred_data)
```



- The aesthetic mapping is inherited from the top level `ggplot` call to the `geom_line`

Plot the model

Option 2: Use the `predict()` function

Summary of general workflow

- **Step 1:** Use `expand_grid` to create a tibble with values for all predictor variables (the columns have to have the exact same name as the original data)
- **Step 2:** Use `predict` to predict response variable with the model using input predictor values from tibble in step 1
- **Step 3:** Add predictions as column to the tibble from step 1
- **Step 4:** Add predictions to the plot using a new `geom_line()` layer based on the tibble from step 3

Analysis of variance (Anova)

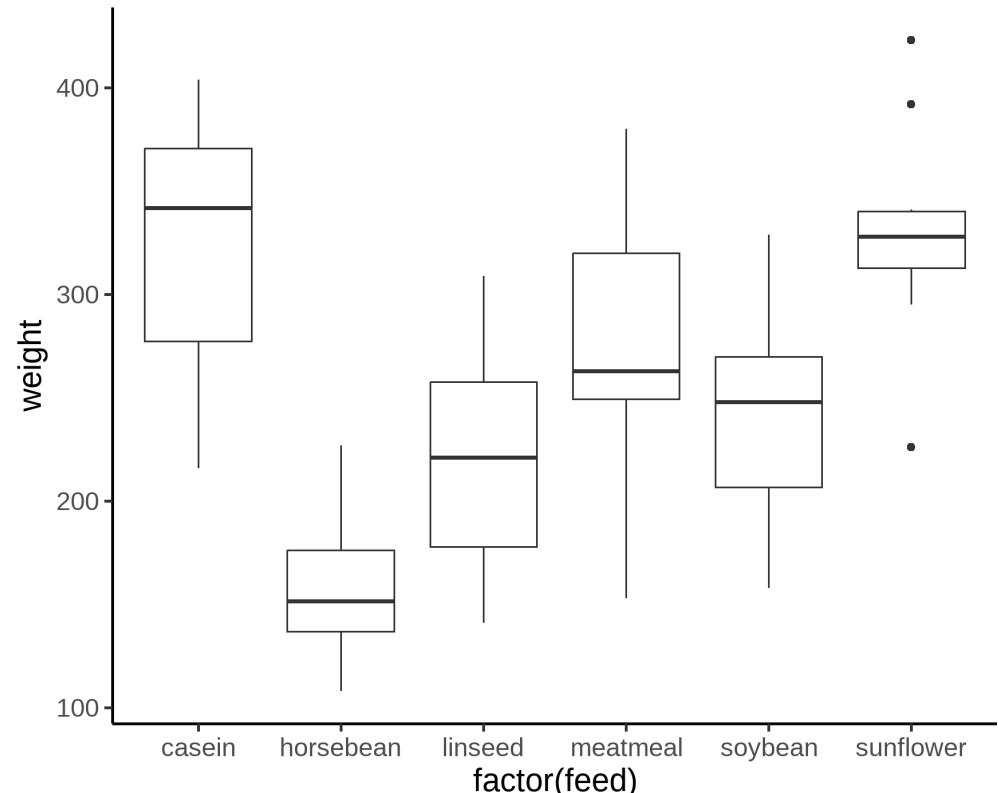
Anova

Only categorical predictors.

Example: Data set `chickwts` about the weight of chickens fed with different diets.

```
chickwts

## # A tibble: 71 × 2
##   weight feed
##   <dbl> <fct>
## 1    179 horsebean
## 2    160 horsebean
## 3    136 horsebean
## 4    227 horsebean
## # ... with 67 more rows
```



Anova

H_1 : The diet has an effect on the weight of chicken.

Fit a linear model with `lm` and test the significance of the predictor:

```
lm_chicken <- lm(weight ~ feed, data = chickwts)
drop1(lm_chicken, test = "F")
## Single term deletions
##
## Model:
## weight ~ feed
##      Df Sum of Sq    RSS    AIC F value    Pr(>F)
## <none>          195556 574.39
## feed     5     231129 426685 619.78  15.365 5.936e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Removing the predictor `feed` from the model significantly increases the RSS → The model with `feed` explains the data better than the model without `feed`, so the effect of `feed` on the chicken weight is significant.

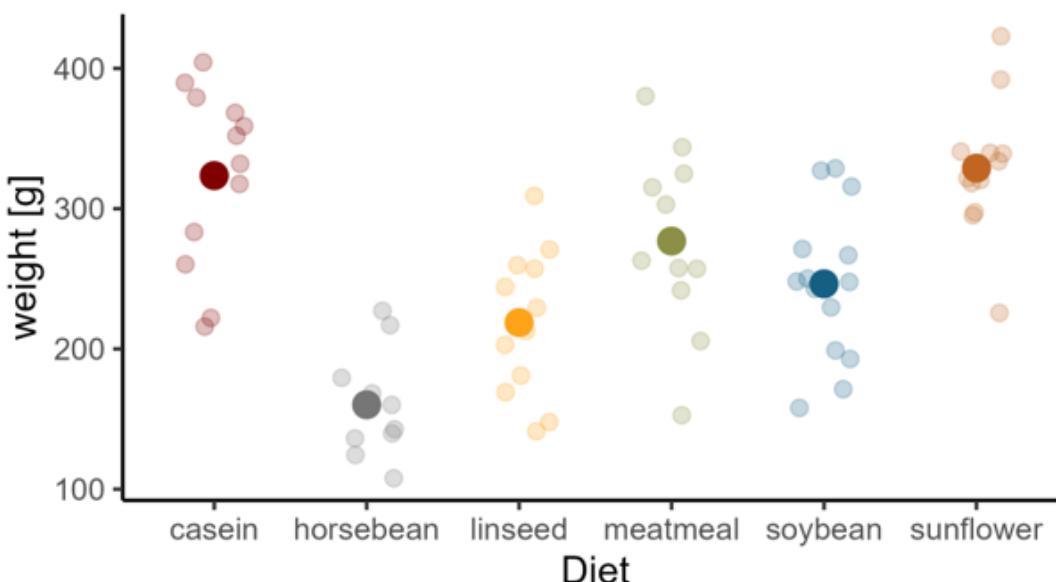
Extracting model coefficients

```
summary(lm_chicken)
##
## Call:
## lm(formula = weight ~ feed, data = chickwts)
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -123.909 -34.413     1.571   38.170  103.091
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 323.583   15.834  20.436 < 2e-16 ***
## feedhorsebean -163.383   23.485 -6.957 2.07e-09 ***
## feedlinseed   -104.833   22.393 -4.682 1.49e-05 ***
## feedmeatmeal   -46.674   22.896 -2.039 0.045567 *
## feedsoybean    -77.155   21.578 -3.576 0.000665 ***
## feedsunflower      5.333   22.393   0.238 0.812495
##
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 54.85 on 65 degrees of freedom
## Multiple R-squared:  0.5417,    Adjusted R-squared:  0.5064
## F-statistic: 15.36 on 5 and 65 DF,  p-value: 5.936e-10
```

Extracting model coefficients

Coefficients:

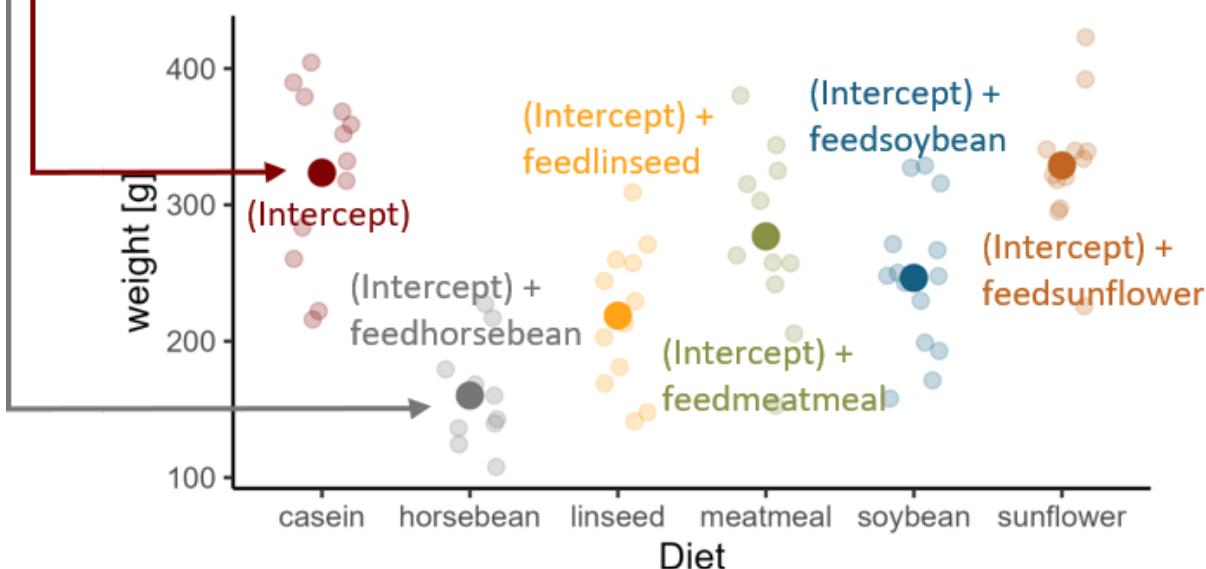
	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	323.583	15.834	20.436	< 2e-16	***
feedhorsebean	-163.383	23.485	-6.957	2.07e-09	***
feedlinseed	-104.833	22.393	-4.682	1.49e-05	***
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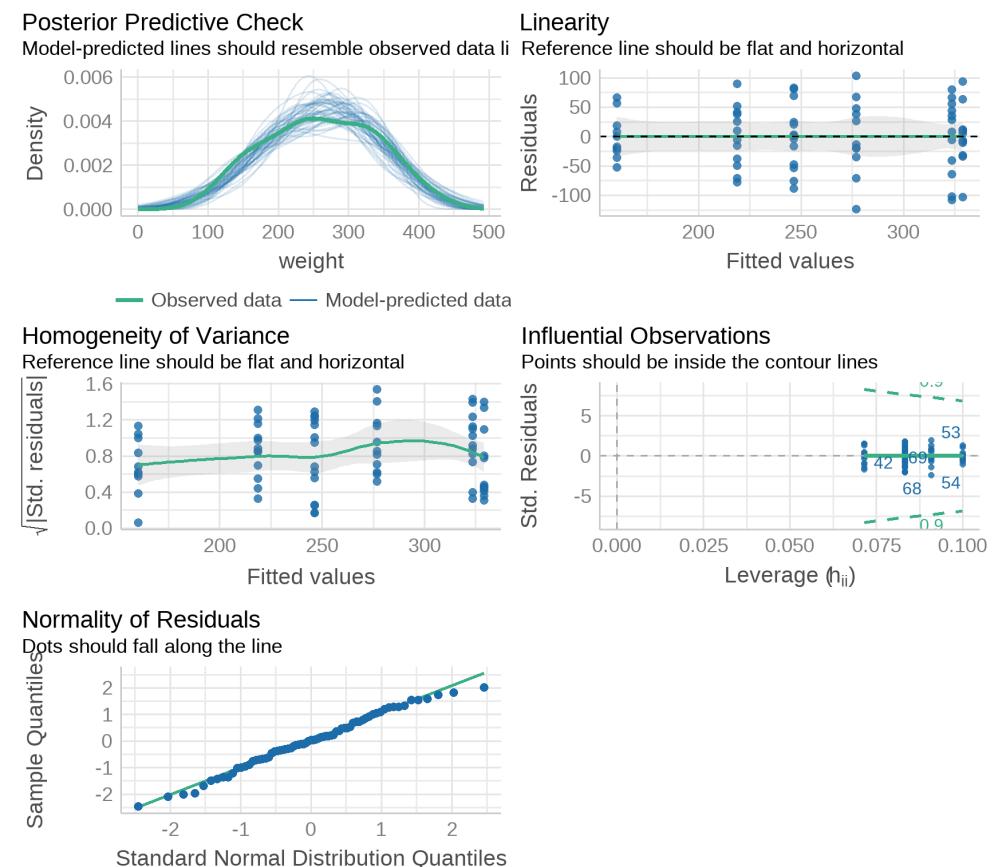


Test model assumptions

Check the assumptions

- Residuals are normally distributed ✓
- Variance is constant (homogeneous) ✓
- There are no strong outliers or very influential observations ✓

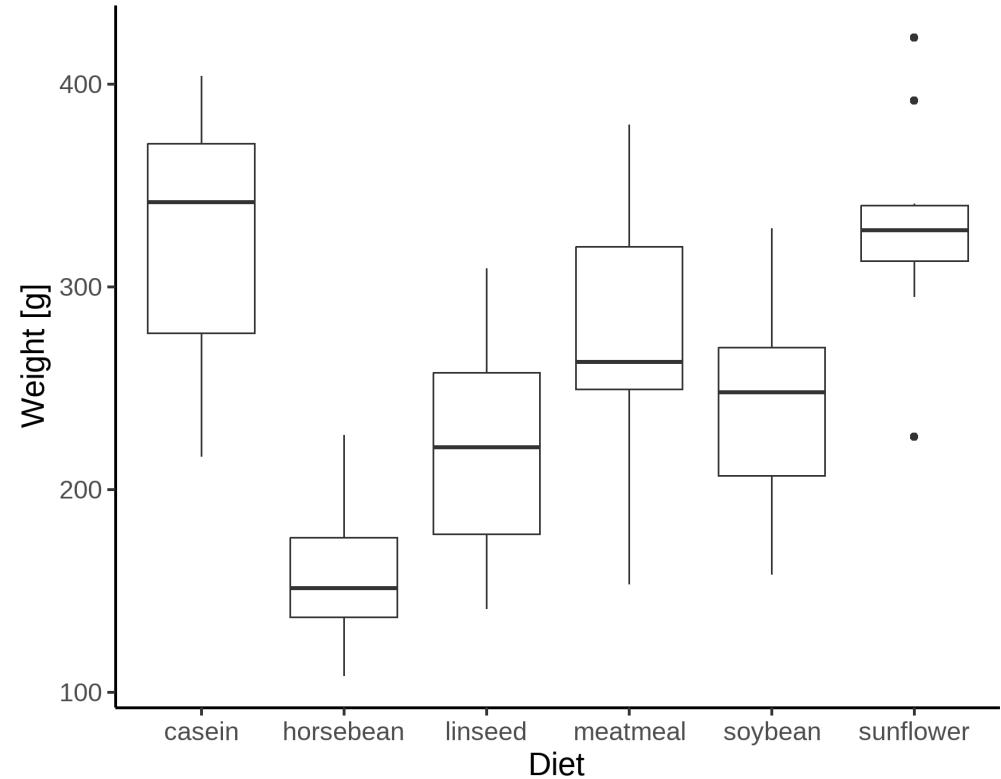
```
performance::check_model(lm_chicken)
```



Plot results

Plot anova results e.g. in a boxplot:

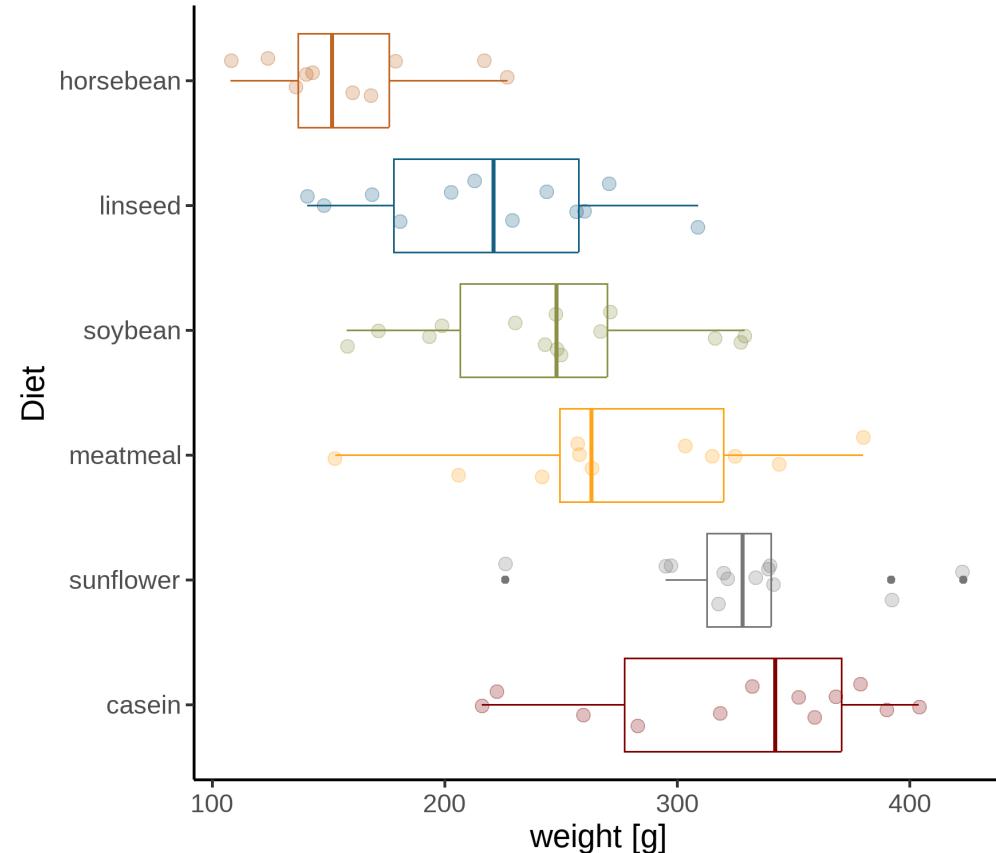
```
ggplot(chickwts, aes(feed, weight)) +  
  geom_boxplot() +  
  labs(x = "Diet", y= "Weight [g]")
```



Plot results

If you want a slightly nicer box plot, you could do something like this:

```
chickwts %>%
  mutate(feed = as.factor(feed)) %>%
  mutate(feed = fct_reorder(feed, -weight)) %>%
  ggplot(aes(
    x = feed,
    y = weight,
    color = feed
  )) +
  geom_boxplot() +
  geom_point(
    size = 3, alpha = 0.25,
    position = position_jitter(width = 0.2,
    seed = 0)
  ) +
  coord_flip() +
  ggsci::scale_color_uchicago() +
  labs(y = "weight [g]", x = "Diet") +
  theme(legend.position = "none")
```



Linear models step by step

Step 1: Explore the data with plots

Step 2: Write down a **question/hypothesis** and think of the **model** to test it

Step 3: Fit the linear model using the `lm` function:

```
lm(formula = Y ~ x1 + x2 + x1:x2, data = dat)
```

- Use `+` for additive effects and `:` for interactions between predictors

Step 4: Check model **assumptions** by looking at the diagnostic plots

```
performance::check_model(mod)
```

- Normally distributed residuals
- Constant variance
- No strong outliers / influential data points

Linear models step by step

Step 5: Check significant variables by conducting F-tests with `drop1`

```
drop1(mod, test = "F")
```

- If the removal of a variable significantly increases the RSS of the model, the predictor is significant

Step 6: Check effect size e.g. in the `summary` table

```
summary(mod)
```

- Extract coefficients from the model with `mod$coefficients`

Step 7: Plot model

- Regression: regression line and scatterplot
- Analysis of covariance: regression lines and scatter plot
- Analysis of variance: boxplots, barplot, mean + sem or similar

Options for model plotting

Option 1: `geom_smooth(method = "lm")`

- Plots a regression line with all interactions between variables
 - only use it if this is what you want to plot

Option 2: extract coefficients and use `geom_abline()`

- Extract slopes and intercepts from the model
 - `mod$coefficients`
- Add a `geom_abline` layer to your plot
 - `geom_abline(slope = your_slope, intercept = your_intercept)`

Options for model plotting

Option 3: Use `predict` function

- This is the most flexible plotting option
- Step 1: Create a new tibble with data to predict from
 - Column names have to be same as predictors of linear model
 - Use e.g. `tidyverse::expand_grid()` to create variable combinations
- Step 2: Predict the response for all value combinations from step 1

```
predict(mod, newdata = pred_data)
```

- Step 3: Add predicted response to tibble from step 1
- Step 4: Add a `geom_line` layer with the new data to your plot

```
ggplot(orig_dat, aes(x = some_x, y = some_y, color = some_col)) +  
  geom_point() +  
  geom_line(data = pred_data)
```

Now you

Task 2: Linear models with the penugin data set

Find the task description [here](#)