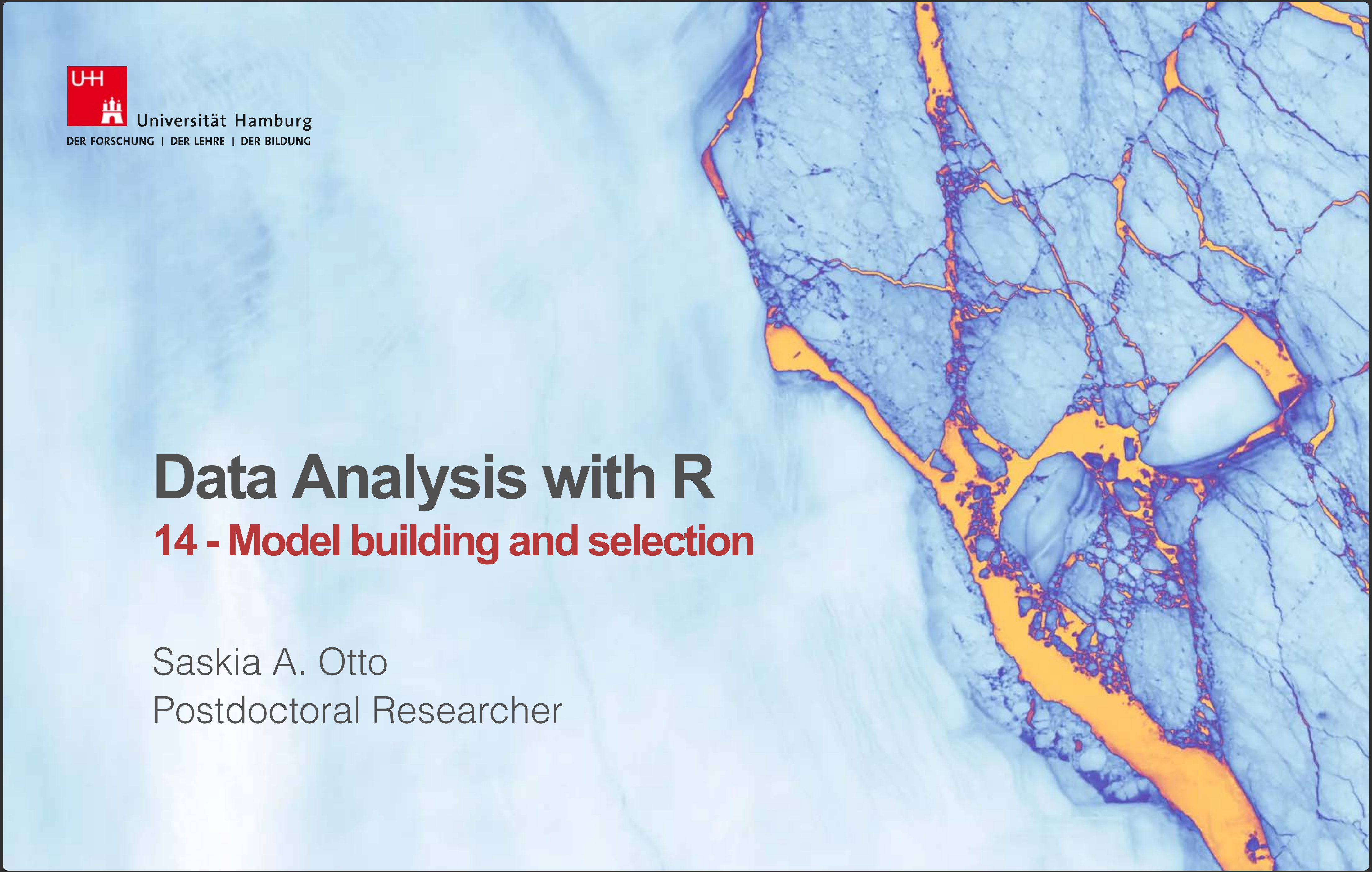
Marine Data Science



Universität Hamburg
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Data Analysis with R

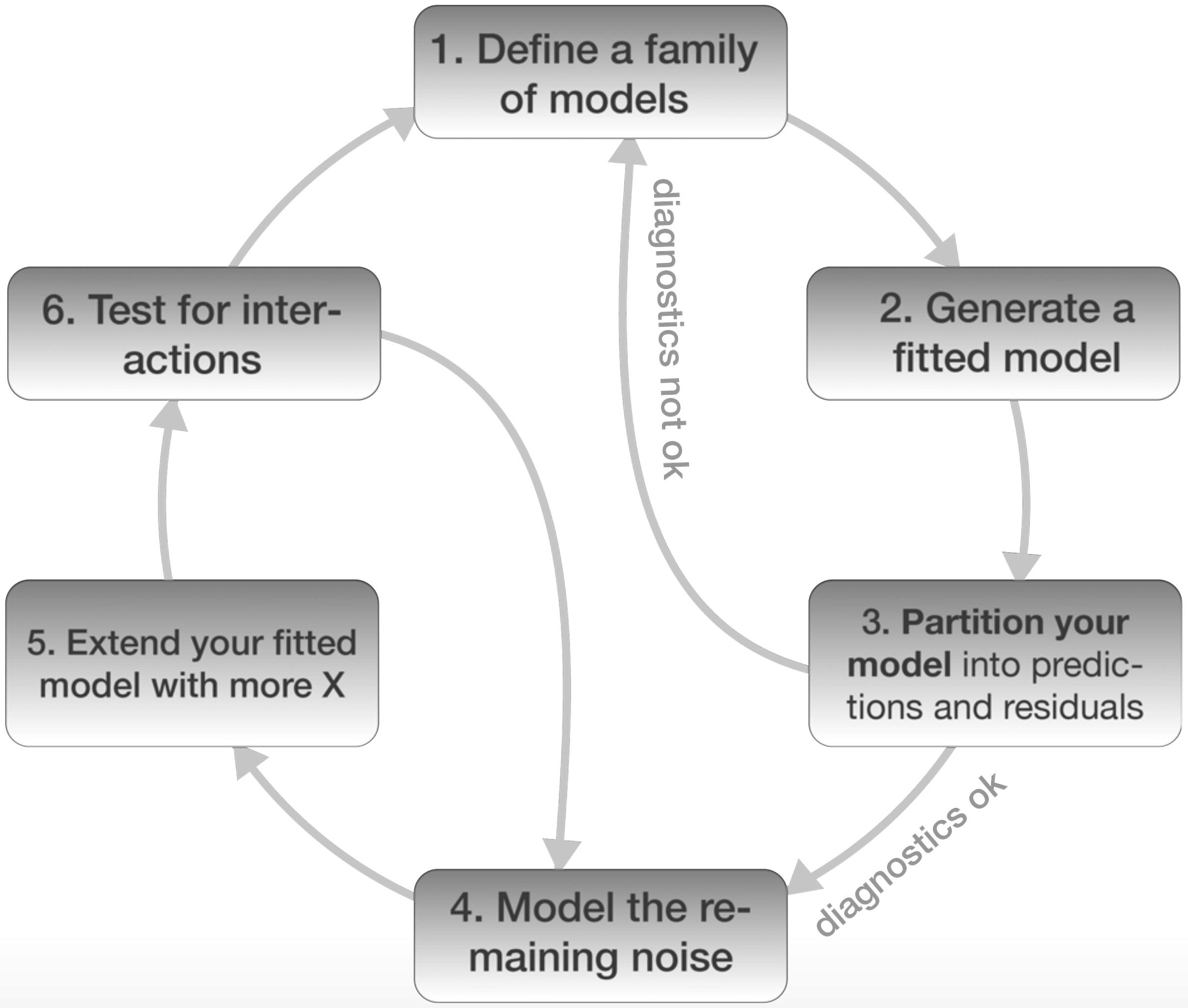
14 - Model building and selection

Saskia A. Otto
Postdoctoral Researcher

Statistical Modelling

Model building

Model building in 6 steps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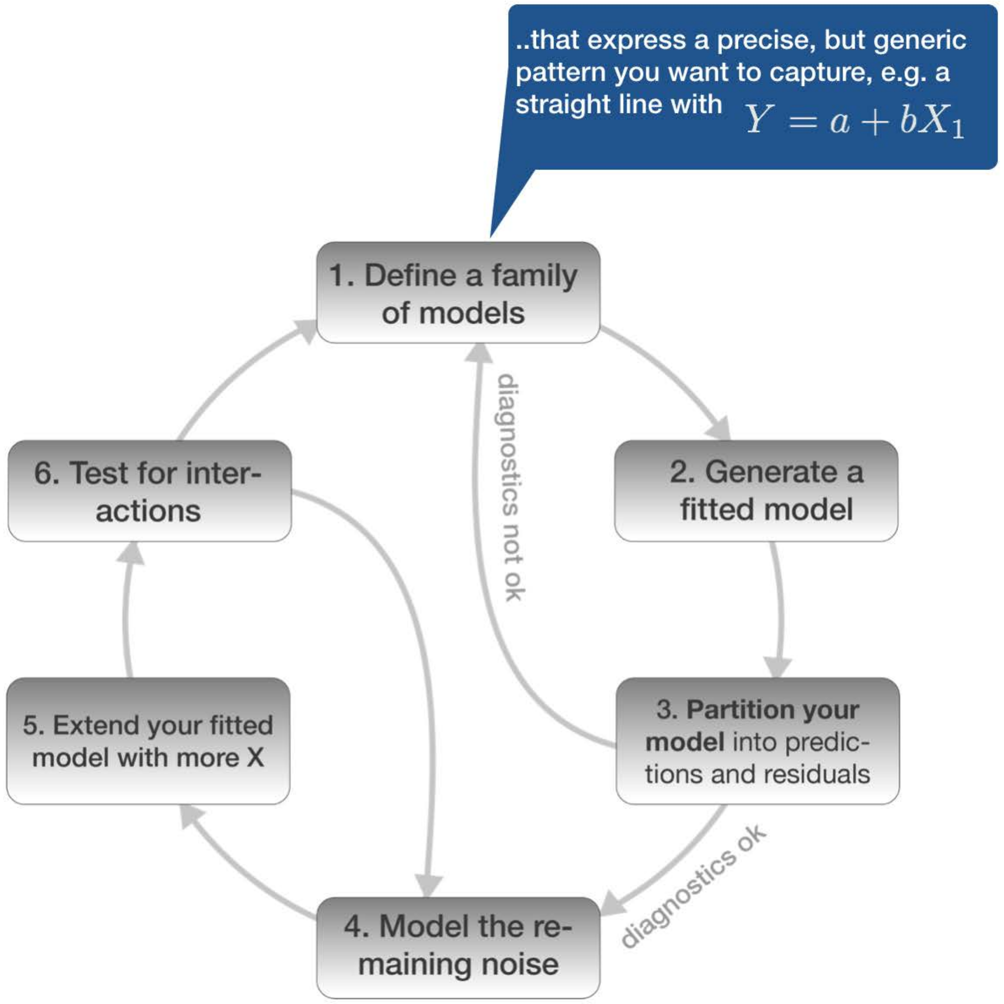
diagnostics not ok
diagnostics ok
4. Model the remaining noise
5. Extend your fitted model with more X
6. Test for interactions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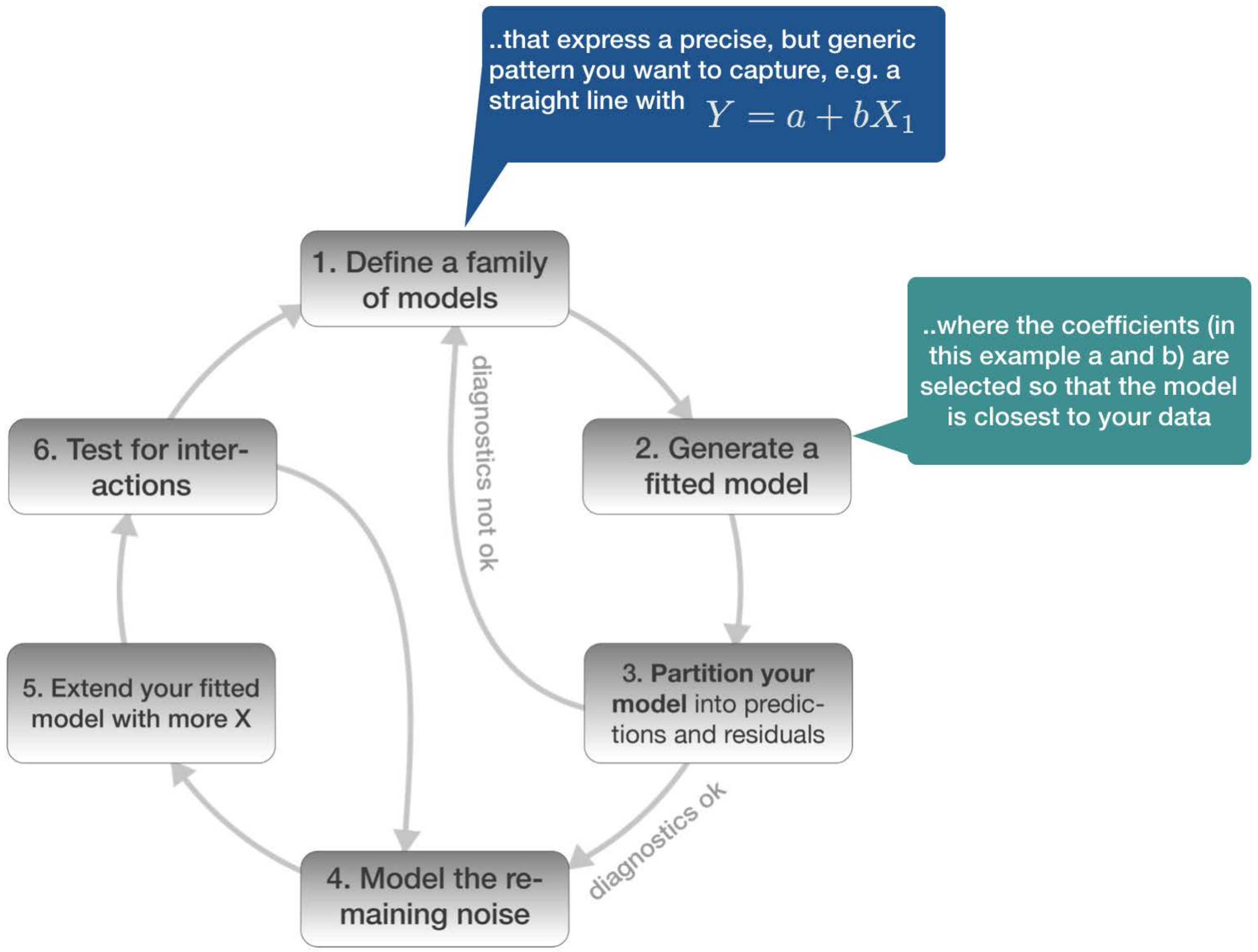
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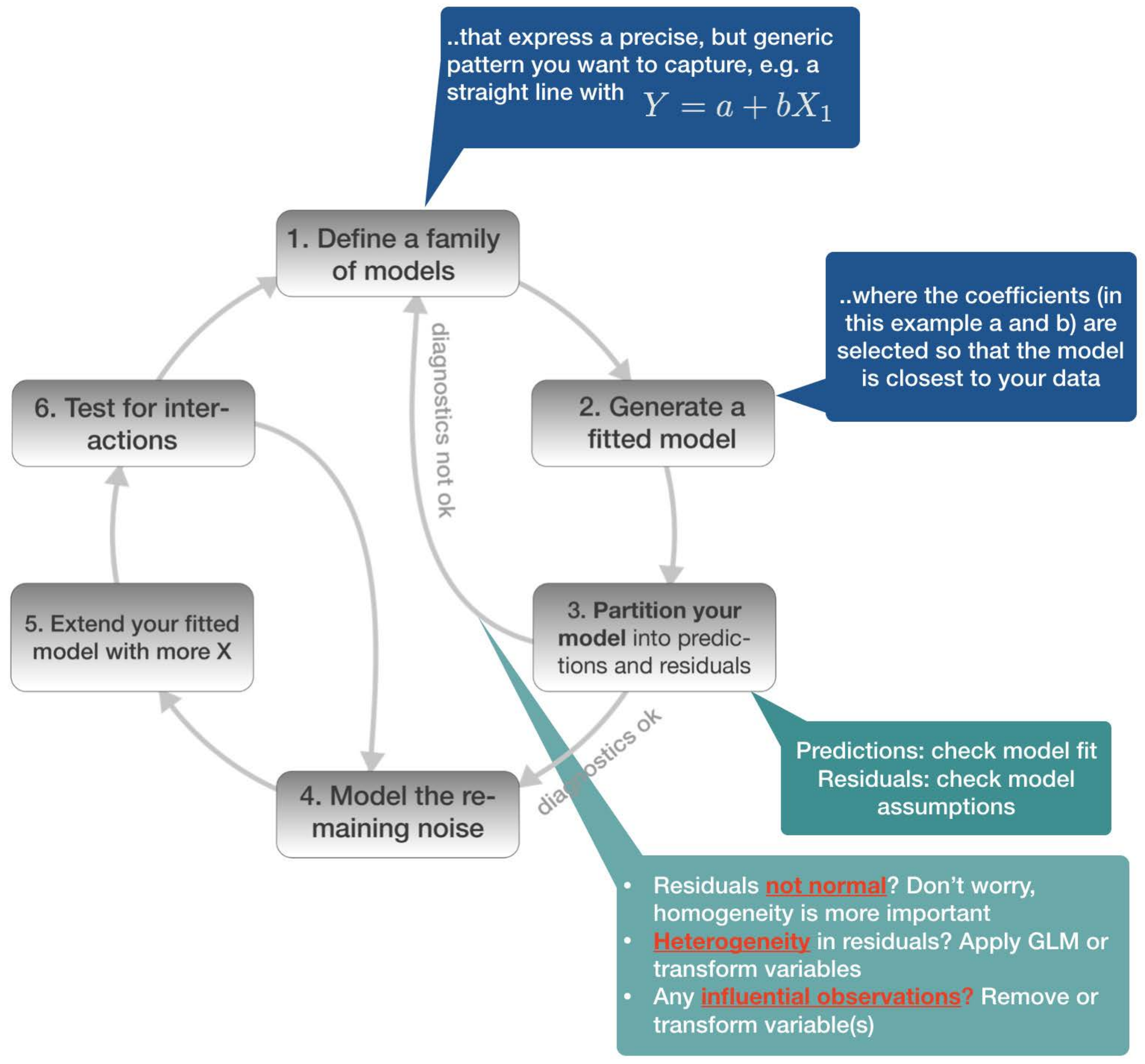
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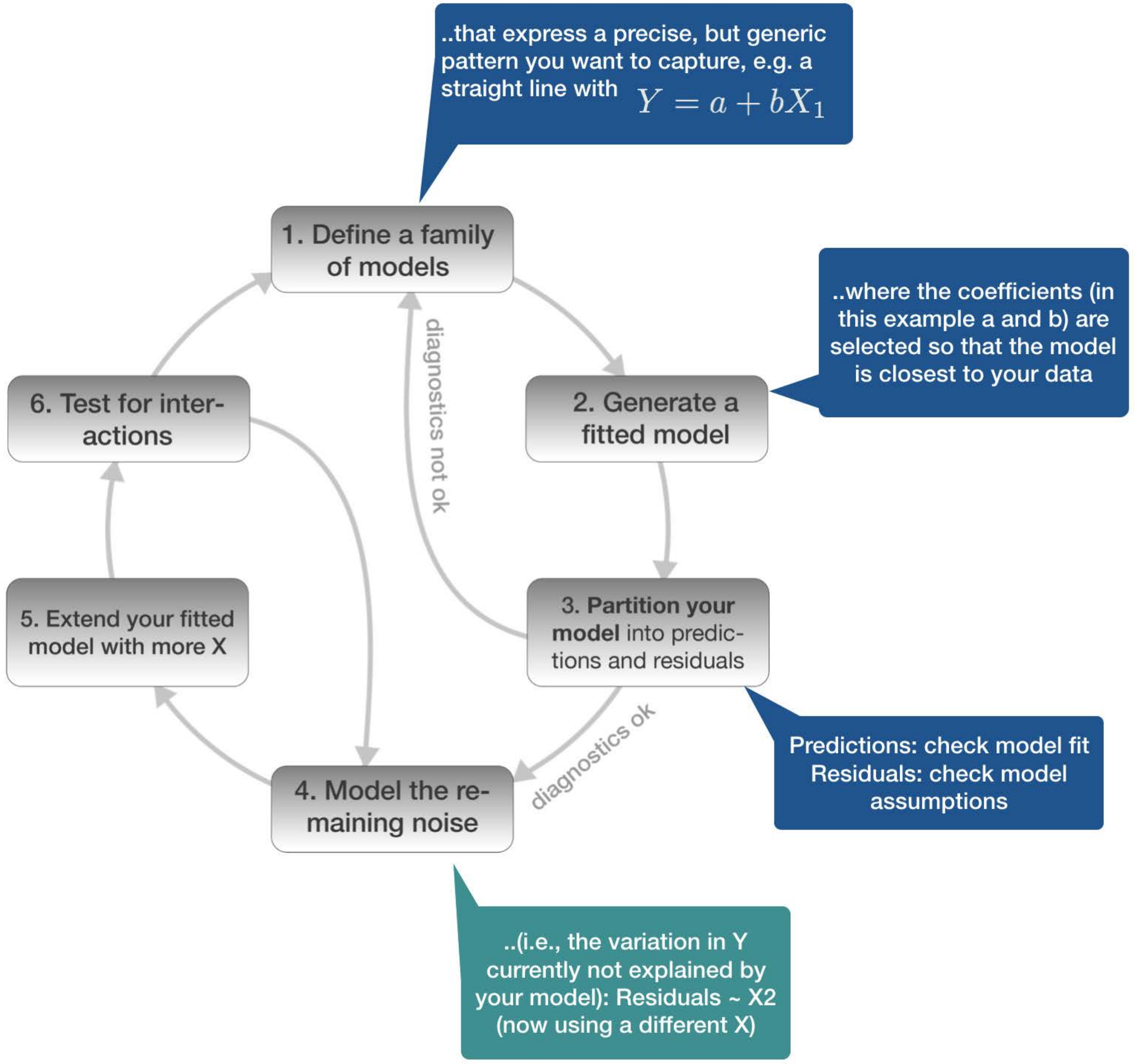
• Residuals not normal? Don't worry, homogeneity is more important
• Heterogeneity in residuals? Apply GLM or transform variables
• Any influential observations? Remove or transform variable(s)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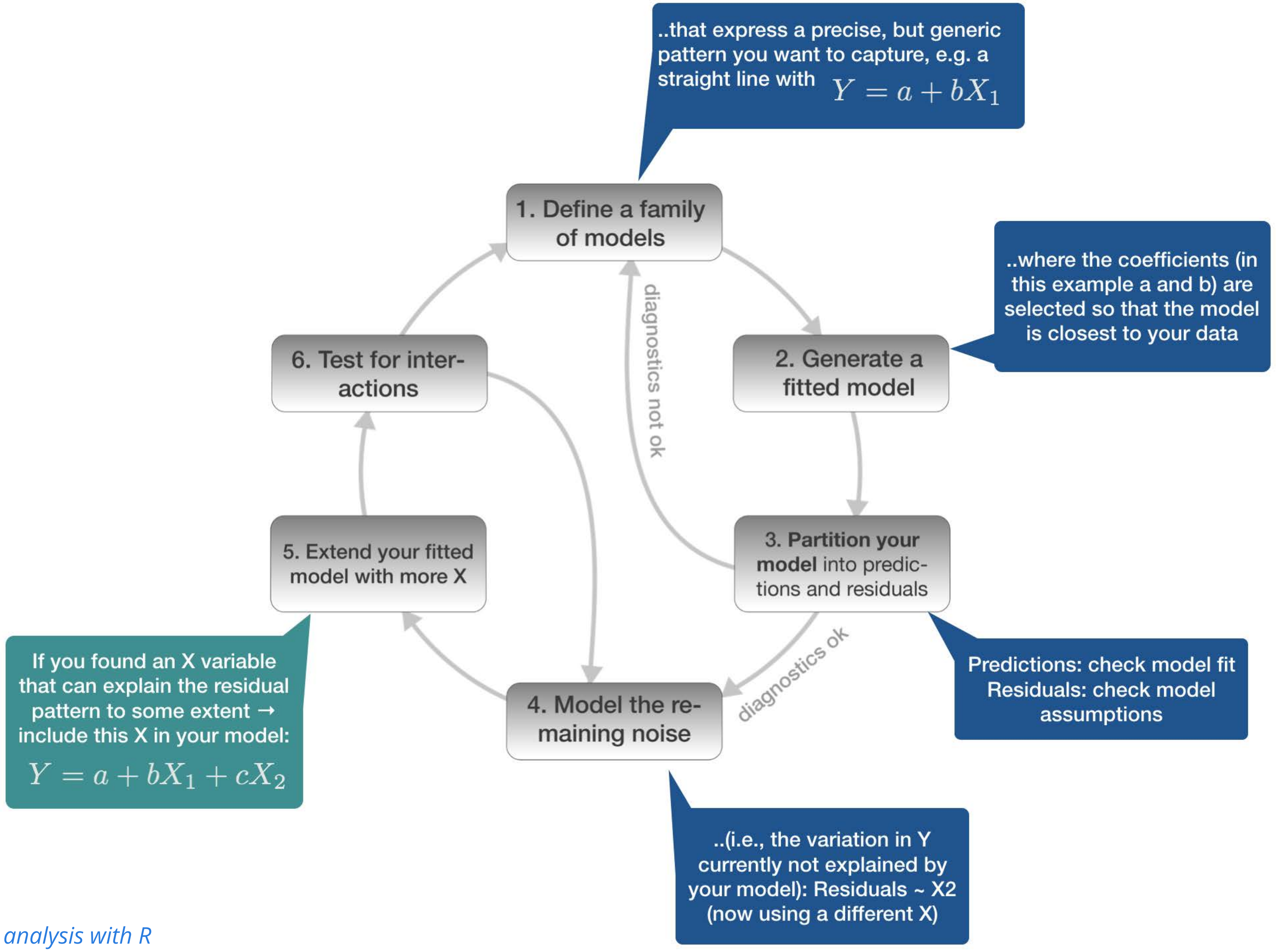
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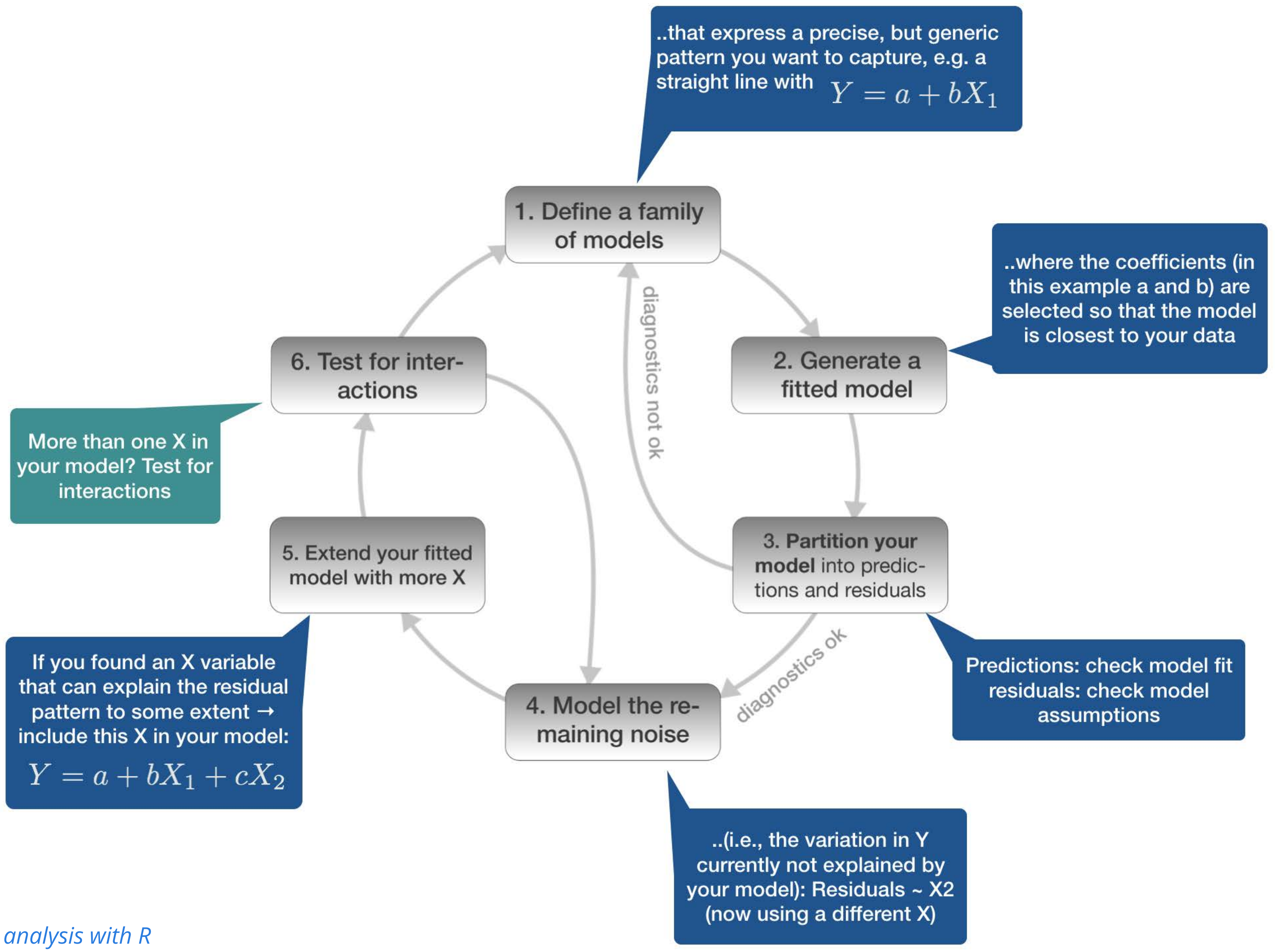
6. Test for interactions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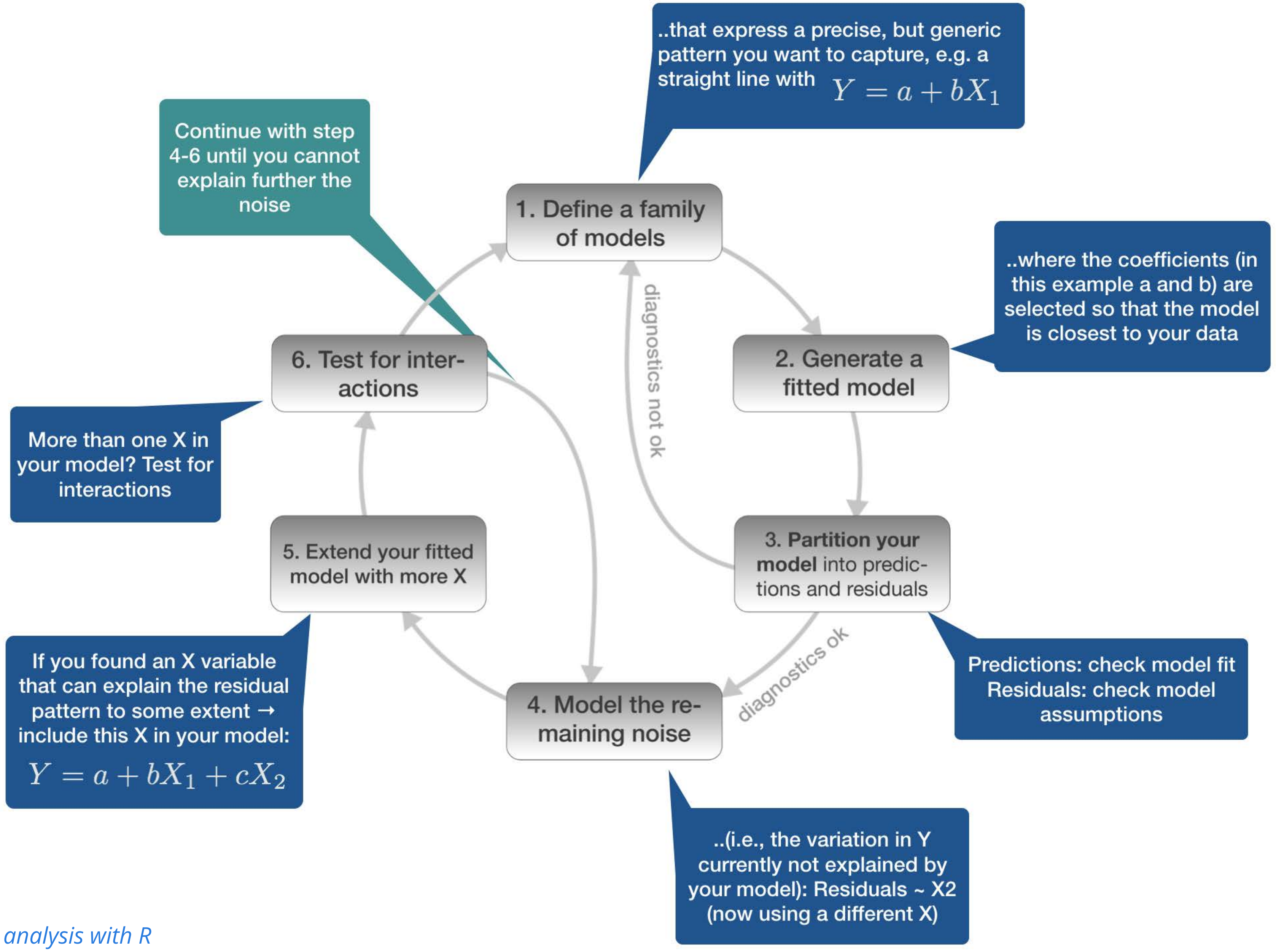
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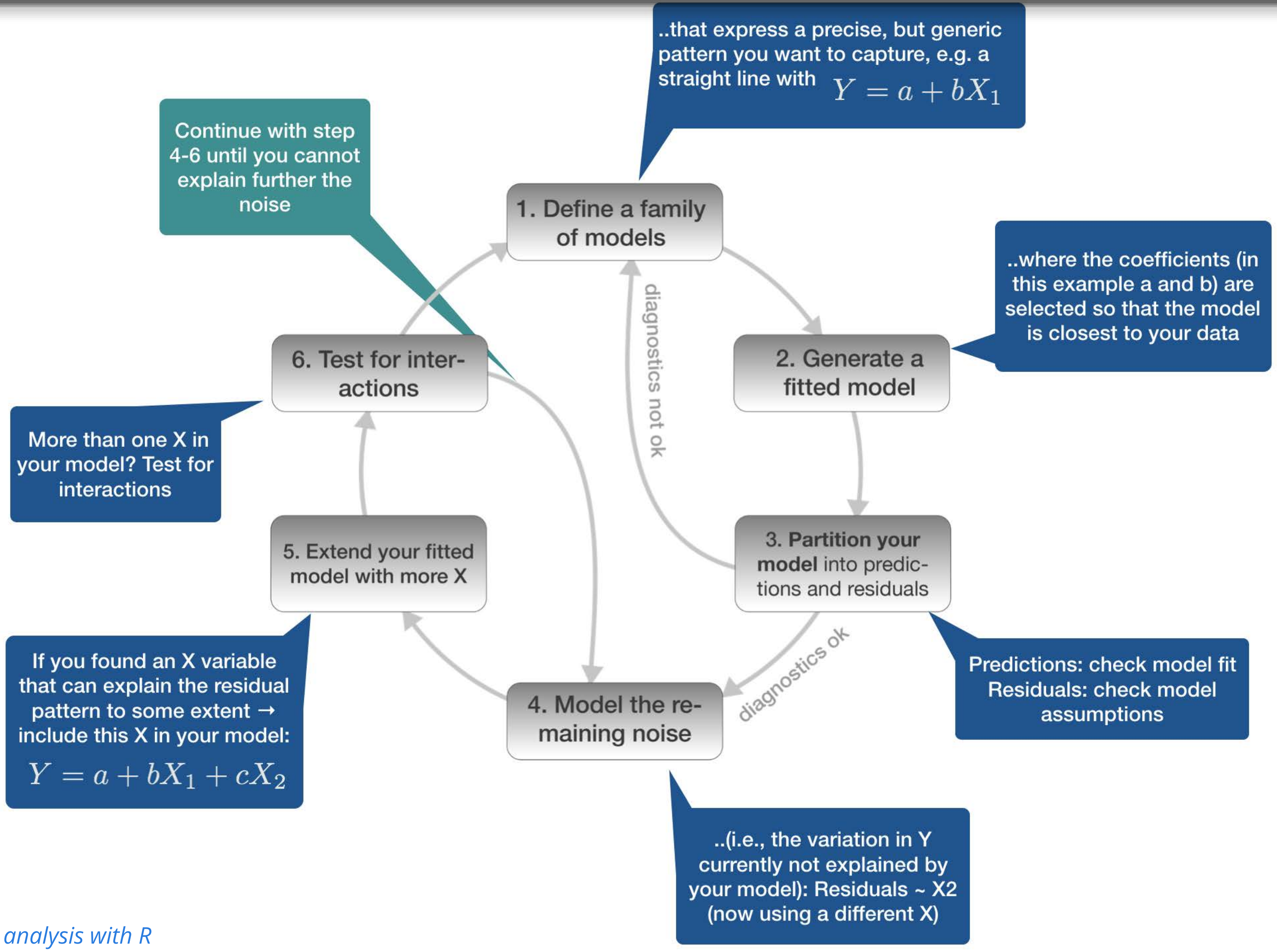
4. Model the re-maining noise
..(i.e., the variation in Y currently not explained by your model): Residuals ~ X2 (now using a different X)

NOTE: You can do step 1-6 also with different model families, compare them and select the one that fits best.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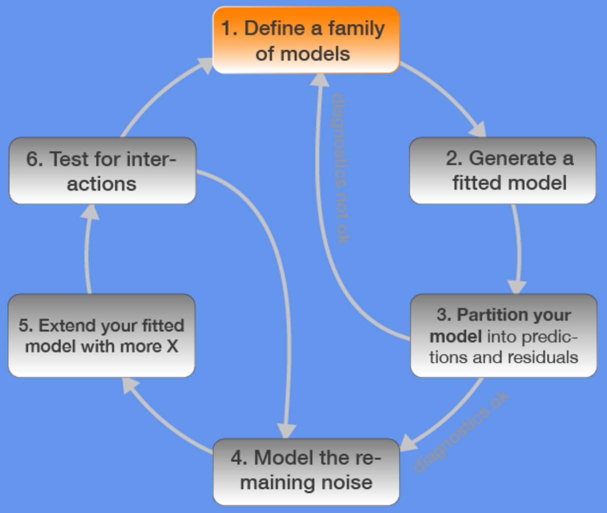
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1. Defining the model family

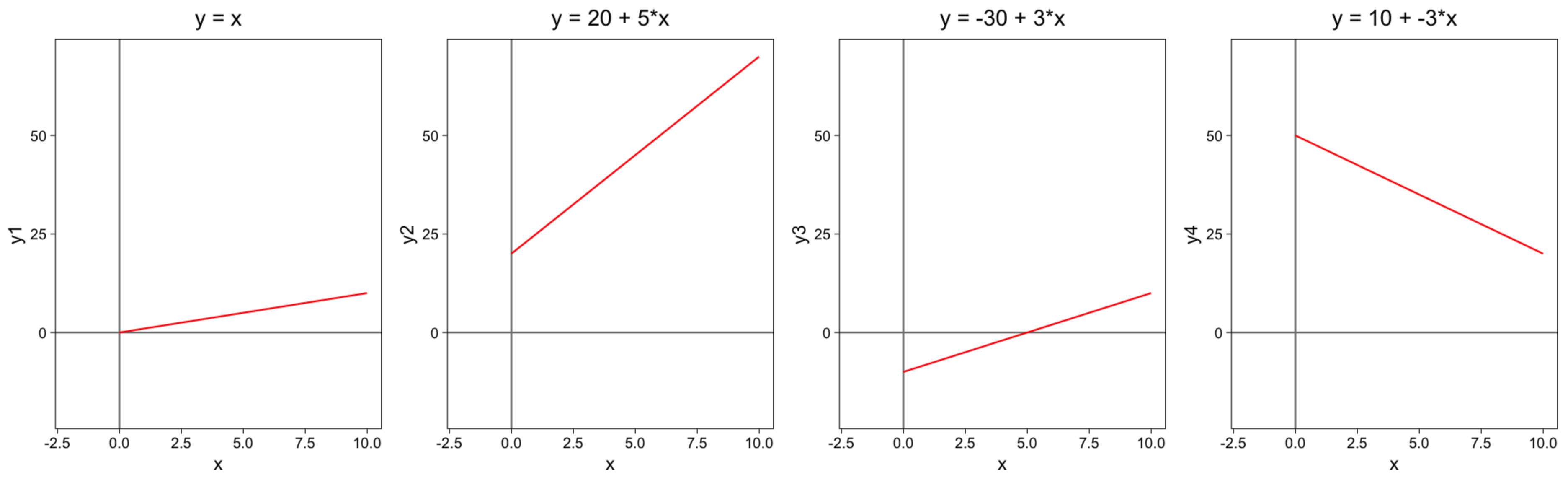
Aim

You want to find the function that best explains Y

$$Y_i = f(\mathbf{X_i}) + \epsilon_i$$

Note:
X can be also a vector of several explanatory variables.

The function for a straight line is $Y = a + bX$

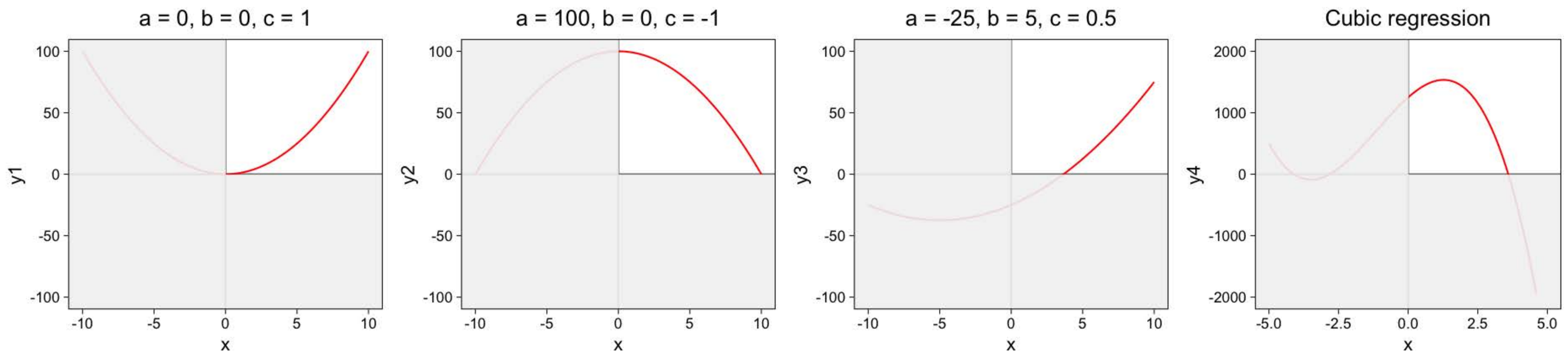


Where *y* is the dependent variable, *a* is the intercept, which is the value at which the line crosses the y-axis (when x is zero), *b* is the coefficent for the slope, and *x* is the independent variable.

Quadratic relationships $Y = a + bX + cX^2$

When the effect of an explanatory variable X changes with increasing or decreasing values of X a model with polynomial terms might be a better option.

The quadratic dependence has three parameters and so can produce a variety of parabolas.



a controls how quickly the parabola increases with X. If it is positive the parabola goes up and is trough-shaped, a negative value of a inverts the parabola. The parameter **c** controls the height of the parabola and the value of **b** controls the sideways displacement of the parabola.

Taylor's theorem

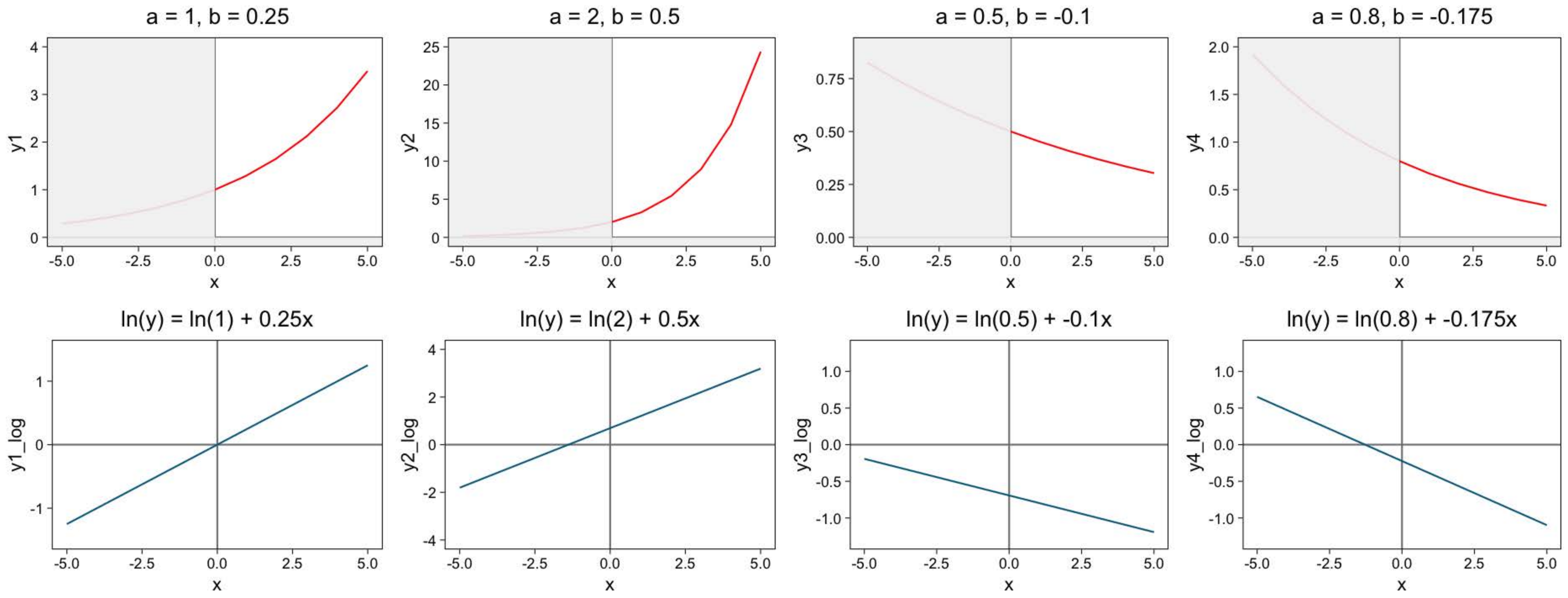
Brook Taylor

- Taylor's theorem says that you can approximate any smooth function with an infinite sum of polynomials.
- You can use a polynomial function to get arbitrarily close to a smooth function by fitting an equation like $Y = a + bX + cX^2 + dX^3 + eX^4$
- R provides helper functions that produce orthogonal (i.e. uncorrelated) polynomials
  - `poly(X, degree = 4)` → problem: outside the data range of the data predictions shoot off to +/- Inf
  - alternative: use the natural spline with `splines::ns(X, df = 4)`

source image: Wikipedia (under CCO licence)

Exponential growth or decay

Curves following exponential growth or decay occur in many areas of biology. A general exponential growth is represented by $Y = a * e^{bX}$, a decay by $Y = a * e^{-bX}$.



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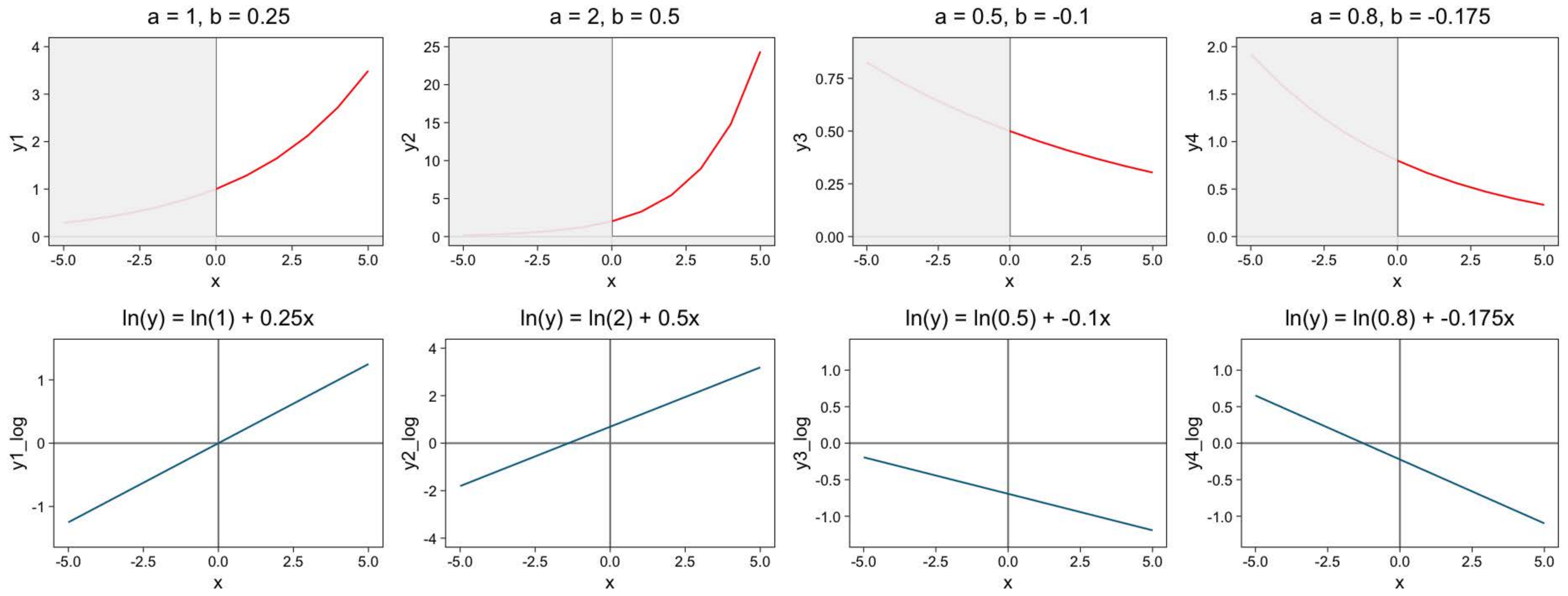
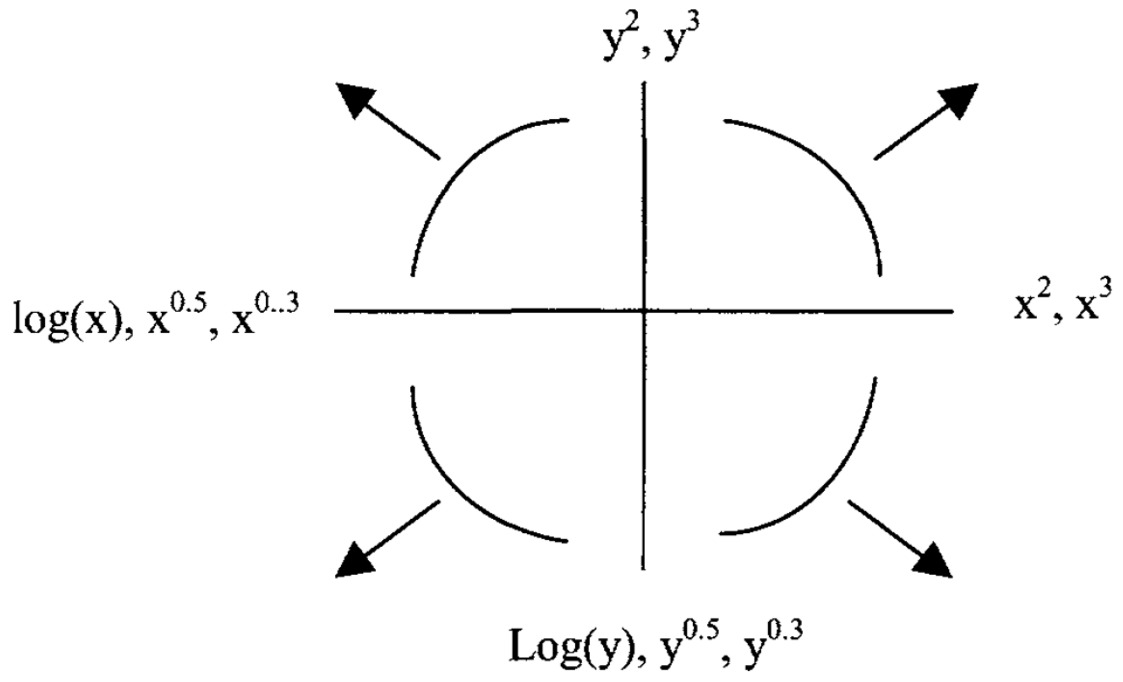


Since the natural log is the inverse function of an exponential function, ln(exp(x)) = x, an exponential curve can be changed into a linear relationship by taking the natural log of both sides of the equation.

Linearizating relationships through transformations



y^2, y^3
$\log(x), x^{0.5}, x^{0..3}$
x^2, x^3
$\mathrm{Log}(y), y^{0.5}, y^{0.3}$

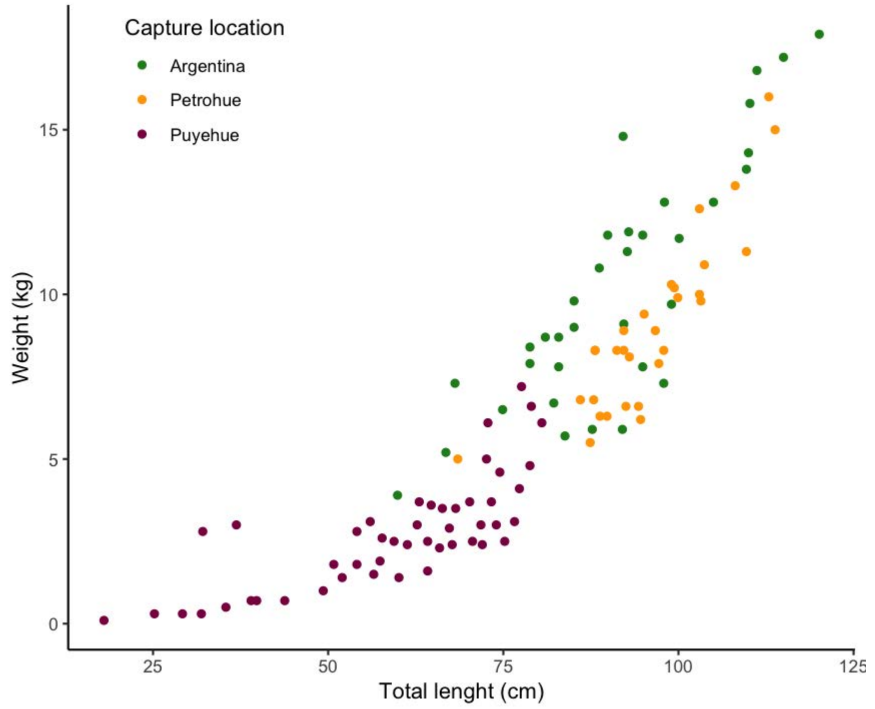
Figure 4.17. Mosteller and Turkey's bulging rule. When the arrow points downwards, y should be made smaller; if it points upwards, it should be increased. If the arrow points towards the left, x should be made larger, etc. See also Fox (2002a).

source: Zuur et al., 2007 (Chapter 4)

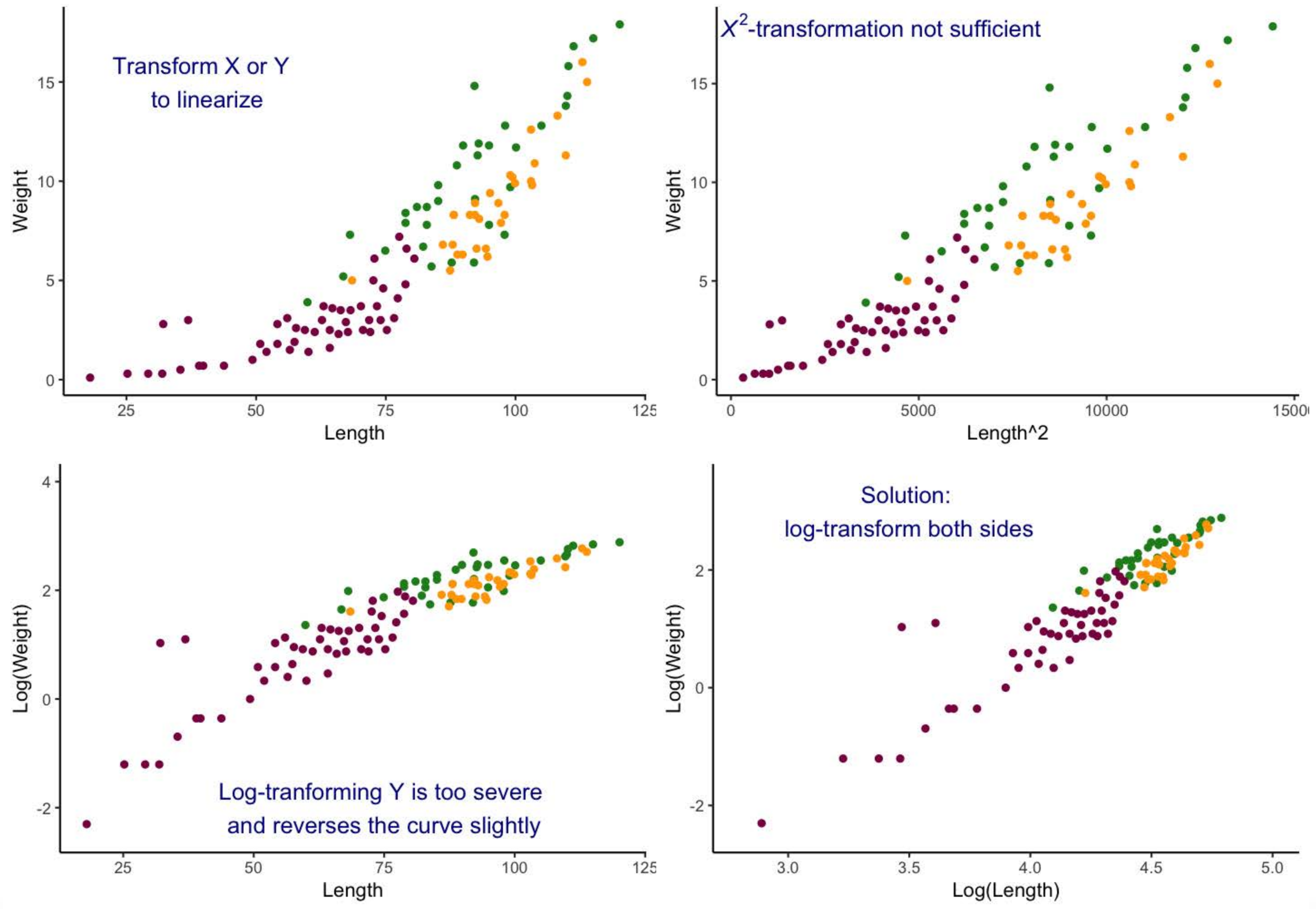
Example: Weight ~ Length relationship

A typical example for a linear relationship, which cannot be described by linear graph, is in marine biology the weight-length relationships. For most species, it will follow a 2 parameter power function: $W = aL^b$

Lengths and weights for Chinook Salmon from three locations in Argentina (data is provided in the FSA package).

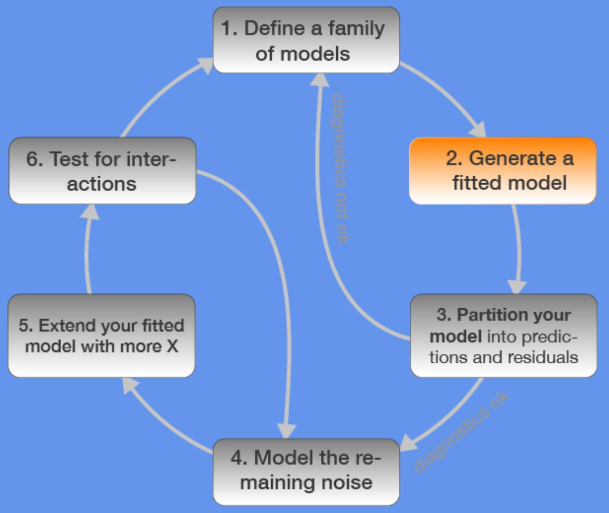


Applying the bulging rule



General rule for common transformations

- **Square root** transformation: `sqrt()`
  - Count data.
  - Variance is about equal to the mean.
- **Log** transformation: `log()`
  - Variances are not similar or larger than the mean.
  - If the variables contains zeros add a constant (should be a proportionally small value) to each of the observations: `log(X+1)` or `log1p()`
  - to back calculate: `exp(X_log)` or `expm1(X_log)` if 1 was added
- **Arcsine** transformation: `asin()`
  - Percentages and proportions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2. Generate a fitted model

Once you defined the model family

- you can estimate the coefficients (in an iterative process) yourself
- or you select the appropriate R function and the coefficents are automatically estimated.
- The choice of function depends on the model family but also the **data type** and **distribution of Y**:

An overview of common linear models

DATA TYPE Y	DATA TYPE X	DISTRIBUTION Y	R FUNCTION	STATISTICAL MODEL
continuous	continuous	Gaussian	`lm()`	normal linear regression
continuous	categorical	Gaussian	`aov()` or `anova(lm())`	Analysis of Variance (ANOVA)
continuous	both	Gaussian	`lm()`	Analysis of Covariance (ANCOVA)
count	both	Poisson, negative bionomial	`glm()`	log-linear models (Poisson / NB regression)
proportion	both	binomial	`glm()`	binomial logistic regression
binary	both	Bernoulli	`glm()`	logistic regression
categorical (> 2 classes)	both	multinomial	`glm()`	multinomial logistic regression (seldom)
categorical (> 2 classes)	both	Gaussian	`MASS::lda`	Linear Discriminant Analysis

Defining the model family in the R formula

Focus on simple normal linear regression models

1. Straight line: `lm(formula = Y ~ X, data)`
2. Relationship with polynomials:
   - Quadratic: `lm(Y ~ poly(X,2), data)` or `~ splines::ns(X, 2)`
   - Cubic: `lm(Y ~ poly(X,3), data)` or `~ splines::ns(X, 3)`
3. Linearize the relationship:
   - `lm(formula = log(Y) ~ X, data)`
   - `lm(formula = Y ~ log(X), data)`
   - `lm(formula = log(Y) ~ log(X), data)`

Formulas

You can see how R defines the model by using `model_matrix()` from the *modelr* package

```
df <- data.frame(y = c(10,20, 30), x1 = c(5,10,15))
model_matrix(df, y ~ x1)
```

```
## # A tibble: 3 x 2
##   `(Intercept)`    x1
##           <dbl> <dbl>
## 1             1     5
## 2             1    10
## 3             1    15
```

Formulas (cont)

Now with polynomials

```
model_matrix(df, y ~ poly(x1, 2))
```

```
## # A tibble: 3 x 3
##   `(Intercept)` `poly(x1, 2)1` `poly(x1, 2)2`
##           <dbl>          <dbl>          <dbl>
## 1             1      -7.07e- 1          0.408
## 2             1      -9.42e-17         -0.816
## 3             1       7.07e- 1          0.408
```

Categorical X variables

If X is categorical it doesn't make much sense to model $Y = a + bX$ as X cannot be multiplied with b. But R has a workaround:

- categorical predictors are **converted into multiple continuous predictors**
- these are so-called **dummy variables**
- each dummy variable is coded as **0 (FALSE)** or **1 (TRUE)**
- the no. of dummy variables = no. of groups **minus 1**
- all linear models fit categorical predictors using dummy variables

The data

```r
df
```

```
##        y length
## 1    5.3      S
## 2    7.4      S
## 3   11.3      L
## 4   17.9      M
## 5    3.9      L
## 6   17.6      M
## 7   18.4      L
## 8   12.8      L
## 9   12.1      M
## 10   1.1      L
```

The dummy variables

```r
model_matrix(df, y ~ length)
```

```
## # A tibble: 10 x 3
##     `(Intercept)` lengthM lengthS
##             <dbl>   <dbl>   <dbl>
##  1              1       0       1
##  2              1       0       1
##  3              1       0       0
##  4              1       1       0
##  5              1       0       0
##  6              1       1       0
##  7              1       0       0
##  8              1       0       0
##  9              1       1       0
## 10              1       0       0
```

Where did the length class L go?

The data

```
df
```

```
##       y length
## 1   5.3      S
## 2   7.4      S
## 3  11.3      L
## 4  17.9      M
## 5   3.9      L
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```

The dummy variables

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model_matrix(df, y ~ length)
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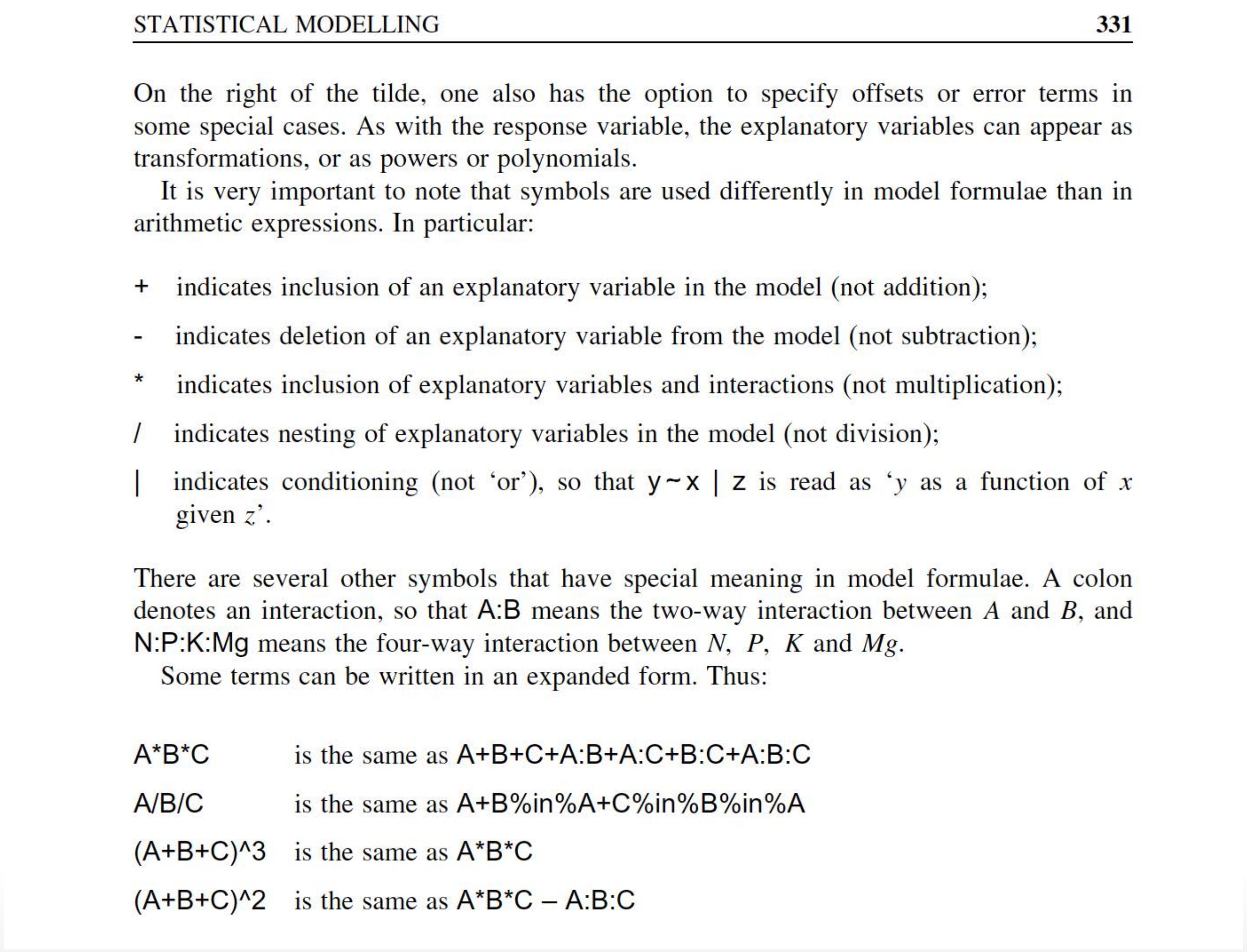
## # A tibble: 10 x 3
##    `(Intercept)` lengthM lengthS
##            <dbl>   <dbl>   <dbl>
##  1             1       0       1
##  2             1       0       1
##  3             1       0       0
##  4             1       1       0
##  5             1       0       0
##  6             1       1       0
##  7             1       0       0
##  8             1       0       0
##  9             1       1       0
## 10             1       0       0
```

L is represented by the intercept !

Overview of model formulae in R



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On the right of the tilde, one also has the option to specify offsets or error terms in some special cases. As with the response variable, the explanatory variables can appear as transformations, or as powers or polynomials.

It is very important to note that symbols are used differently in model formulae than in arithmetic expressions. In particular:

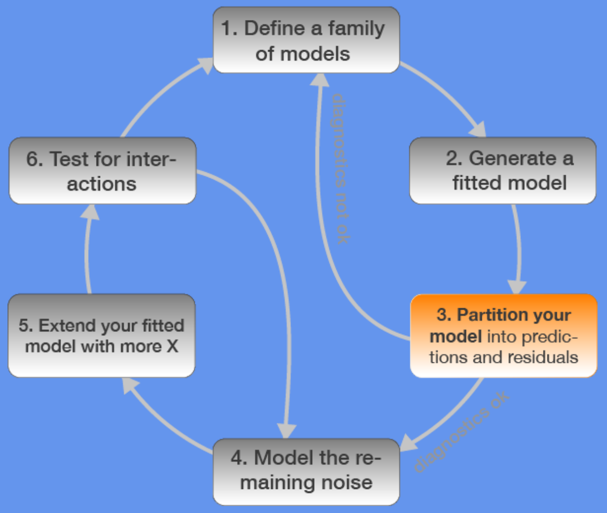
+	indicates inclusion of an explanatory variable in the model (not addition);
-	indicates deletion of an explanatory variable from the model (not subtraction);
*	indicates inclusion of explanatory variables and interactions (not multiplication);
/	indicates nesting of explanatory variables in the model (not division);
|	indicates conditioning (not 'or'), so that `y~x	z` is read as '*y* as a function of *x* given *z*'.

There are several other symbols that have special meaning in model formulae. A colon denotes an interaction, so that `A:B` means the two-way interaction between *A* and *B*, and `N:P:K:Mg` means the four-way interaction between *N*, *P*, *K* and *Mg*.

Some terms can be written in an expanded form. Thus:

`A*B*C`	is the same as `A+B+C+A:B+A:C+B:C+A:B:C`
`A/B/C`	is the same as `A+B%in%A+C%in%B%in%A`
`(A+B+C)^3`	is the same as `A*B*C`
`(A+B+C)^2`	is the same as `A*B*C – A:B:C`

source: Crawley (2007)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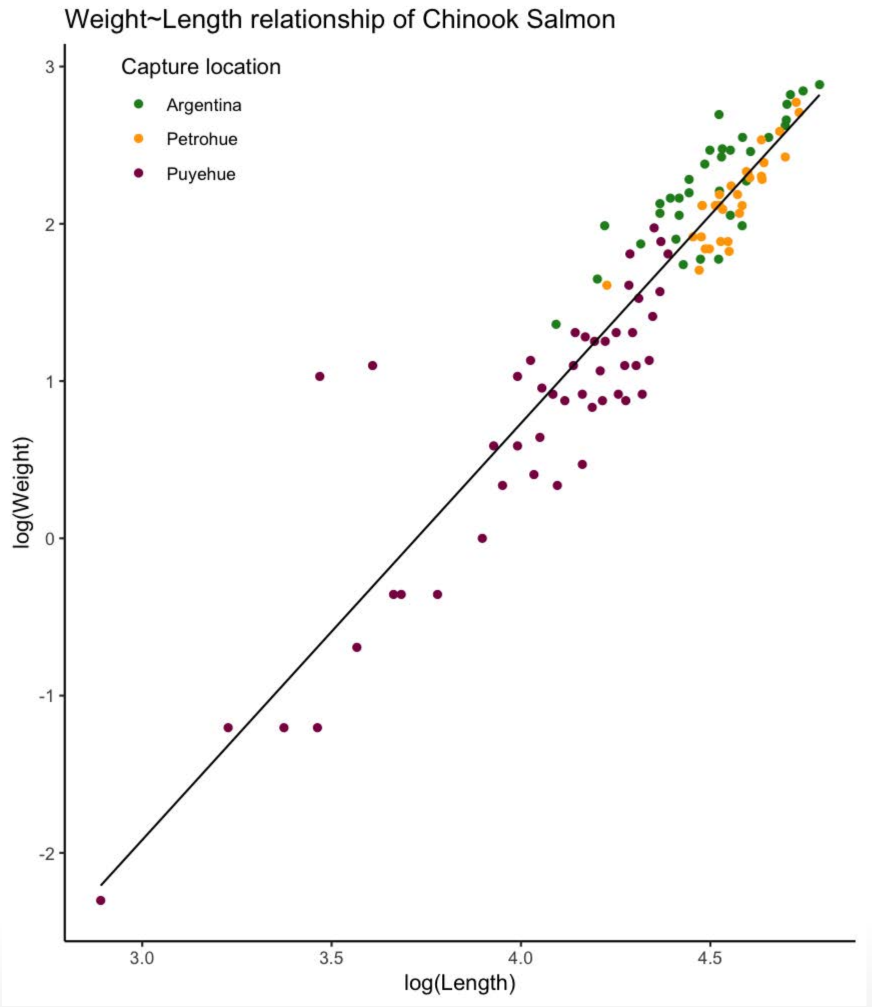
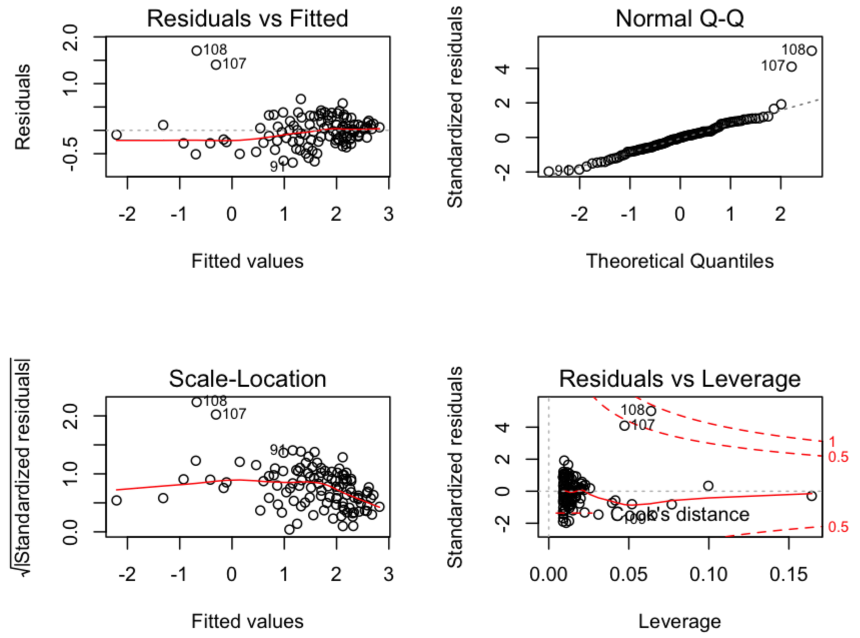
3. Partition your model

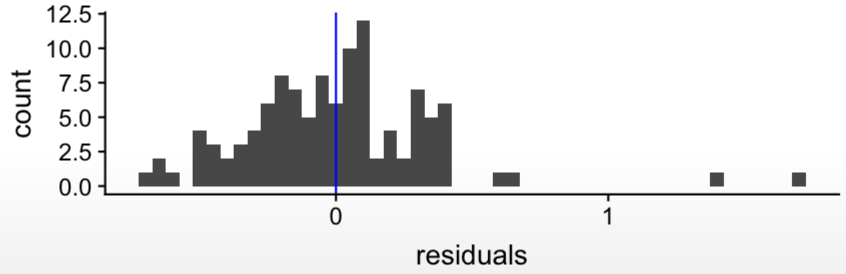
Partition your model into predicted values and residuals

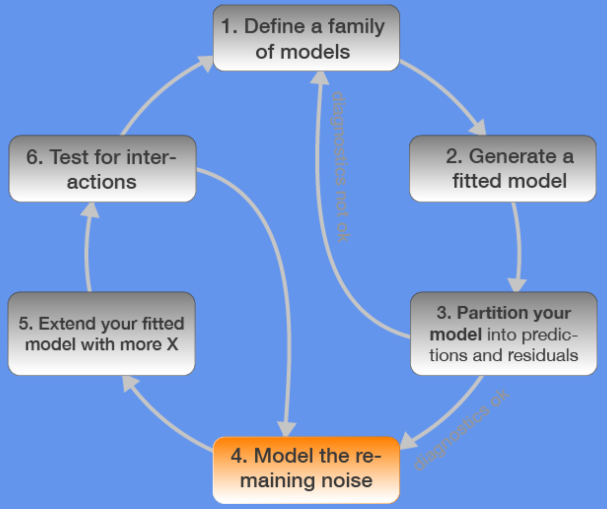
Predicted values: Check **modelfit**



Residuals: Check **assumptions**



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4. Model the remaining noise

2 different ways to understand what the model captures

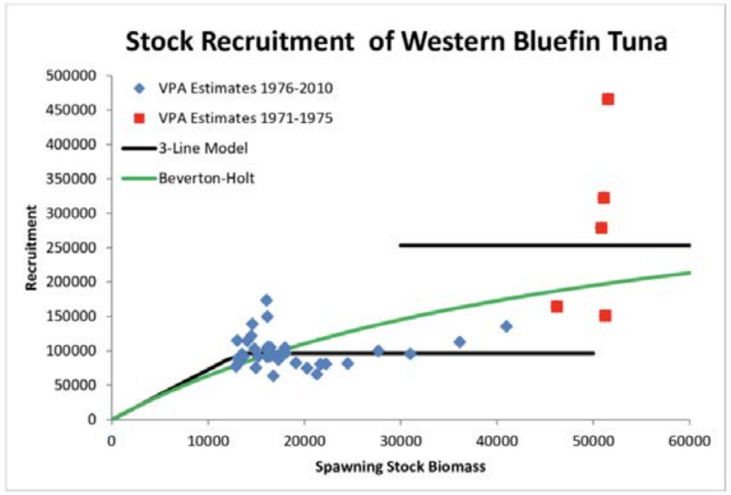
1. Study the model family and fitted coefficients (common in statistical modelling courses).

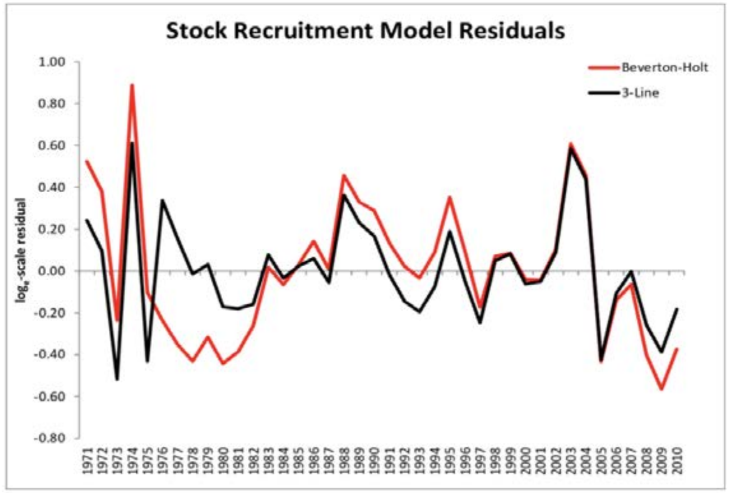
2. Understanding a model by looking at its predictions and what it does not capture (the pattern in the residuals, i.e. the deviation of each observation from its predicted value) (getting more popular these days).

   - Particularly studying the residuals helps to identify less pronounced patterns in the data.

Residual patterns

A typical example where residuals are modelled is in fishery ecology when studying recruitment success:

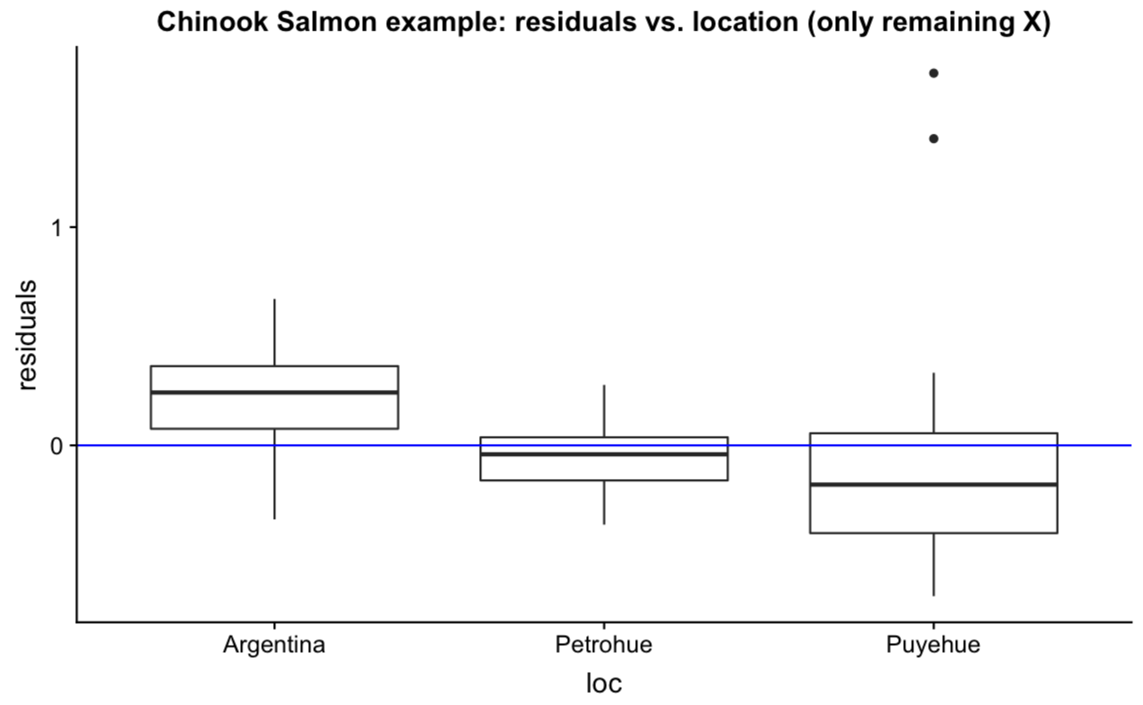




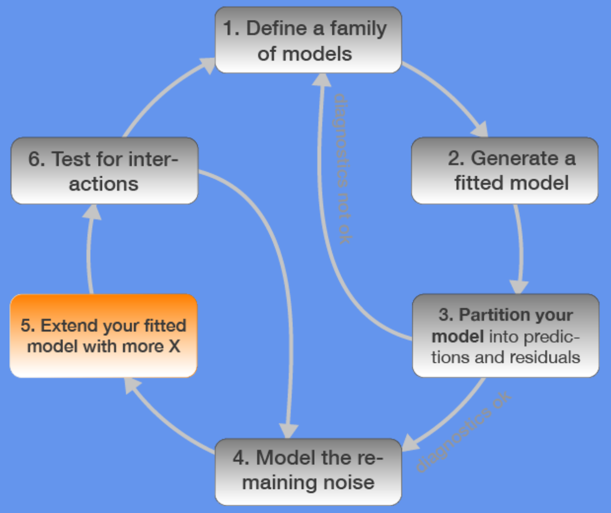
Bluefin Species Group, 2015, Collect. Vol. Sci. Pap. ICCAT, 71(4): 1863-1869

Best practice:

Model the residual ~ every X variable not included in the model



Residuals show a distinct pattern: The model seems to underestimate the weight in Argentina and overestimate in Puyehue.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2. Generate a fitted model
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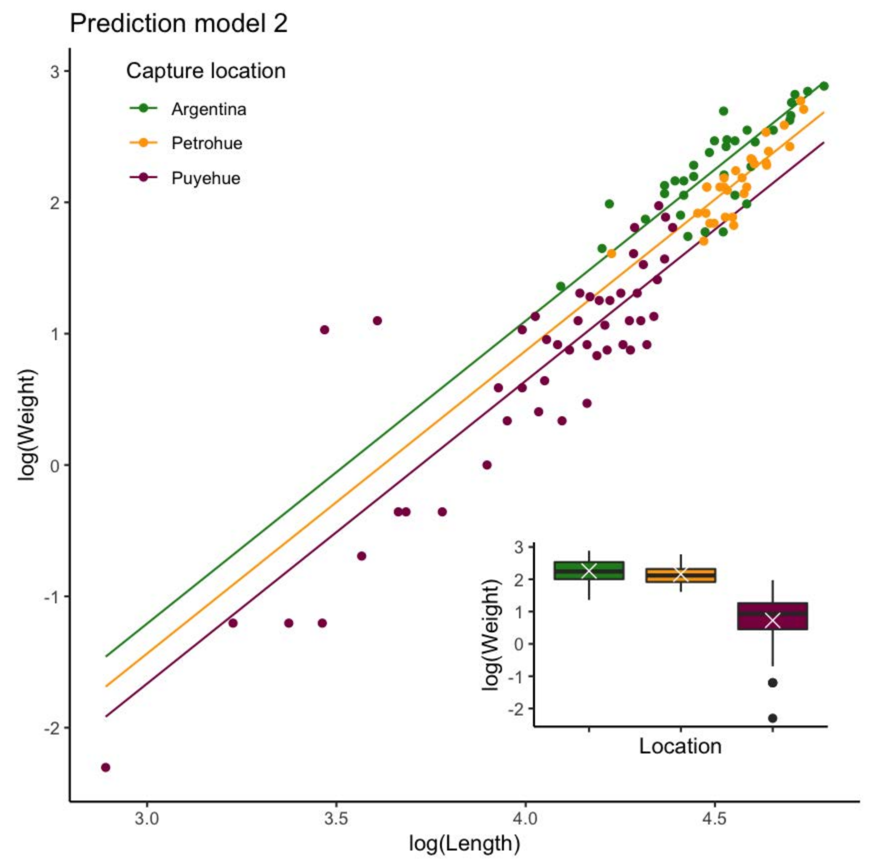
diagnostics not ok
diagnostics ok
4. Model the remaining noise
5. Extend your fitted model with more X
6. Test for interactions

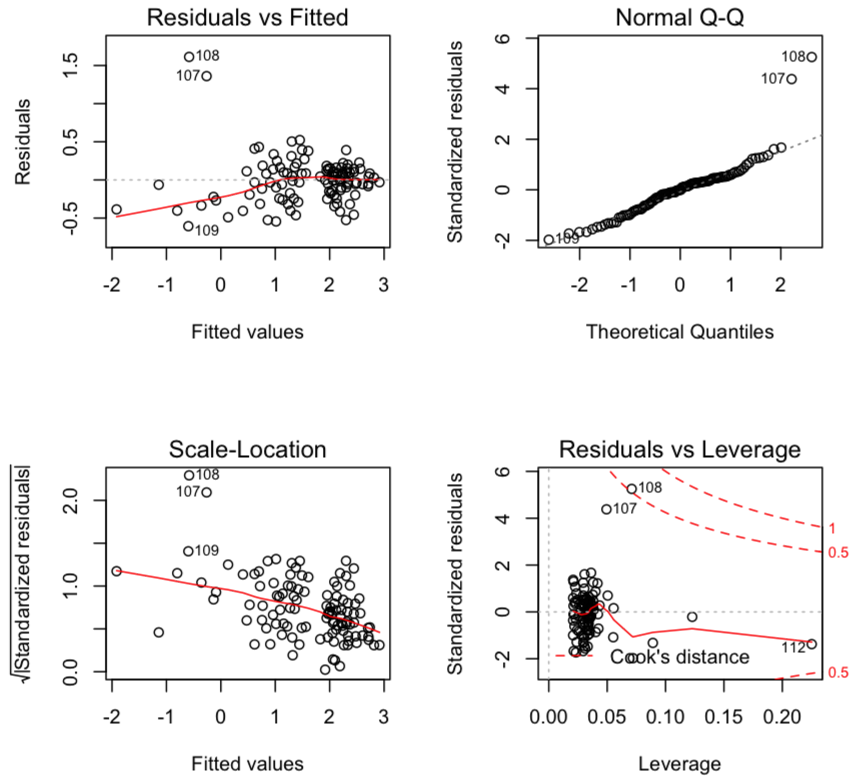
5. Extend your fitted model with more X

Chinook Salmon example: add `loc` as X variable to the model

```r
mod2 <- lm(formula = w_log ~ tl_log + loc, data = ChinookArg)
# alternatively
mod2 <- update(mod, .~. + loc)
```

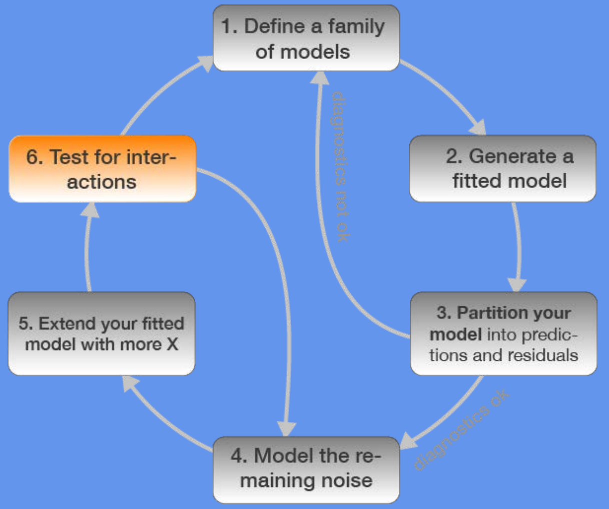
Check modelfit and diagnostics again





```r
summary(mod2)
```

```
##
## Call:
## lm(formula = w_log ~ tl_log + loc, data = ChinookArg)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.60633 -0.19351 -0.00076  0.14352  1.61286
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -8.12169    0.56827 -14.292  < 2e-16 ***
## tl_log       2.30492    0.12563  18.347  < 2e-16 ***
## locPetrohue -0.22813    0.08013  -2.847  0.00528 **
## locPuyehue  -0.45699    0.09231  -4.951 2.74e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3186 on 108 degrees of freedom
## Multiple R-squared:  0.8962, Adjusted R-squared:  0.8934
## F-statistic:   311 on 3 and 108 DF,  p-value: < 2.2e-16
```

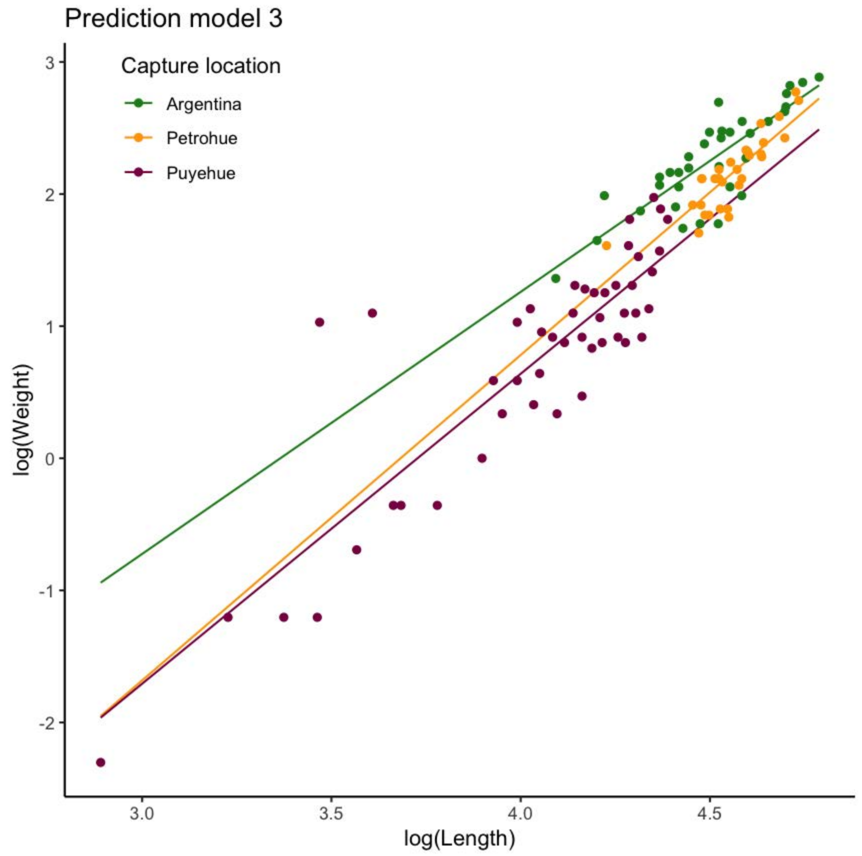

1. Define a family of models
2. Generate a fitted model
3. Partition your model into predictions and residuals
4. Model the remaining noise
5. Extend your fitted model with more X
6. Test for interactions
diagnostics not ok
diagnostics ok

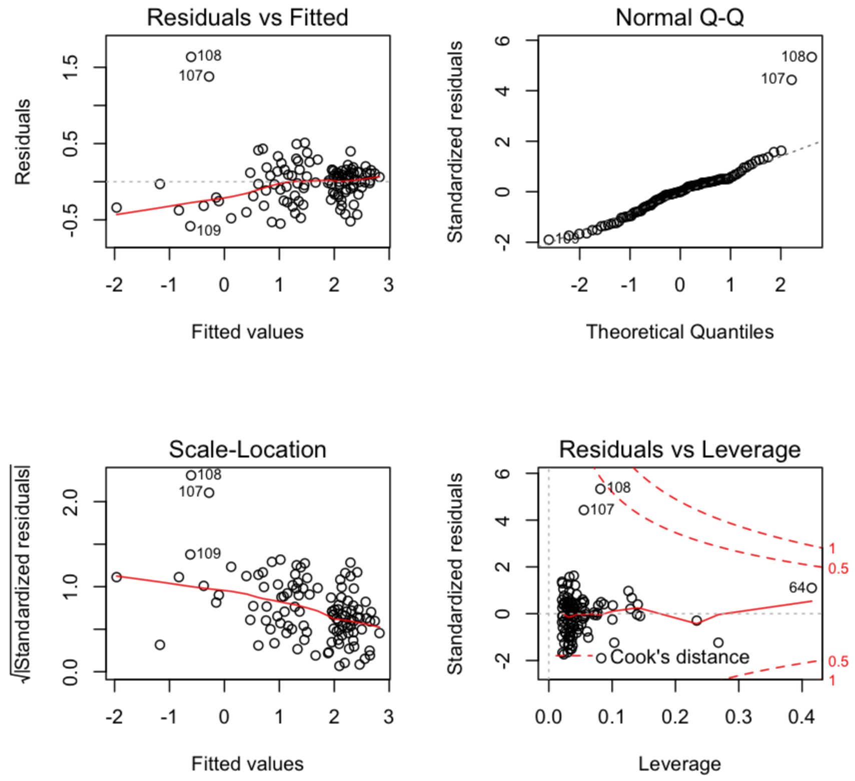
6. Test for interactions

Chinook Salmon example: include `tl_log:loc` interaction

```
mod3 <- lm(formula = w_log ~ tl_log * loc, data = ChinookArg)
# alternatively
mod3 <- update(mod2, .~. + tl_log:loc)
```

Check modelfit and diagnostics again





```r
summary(mod3)
```

```
##
## Call:
## lm(formula = w_log ~ tl_log + loc + tl_log:loc, data = ChinookArg)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.58273 -0.18471 -0.00186  0.13088  1.63620
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)         -6.6750     1.5904  -4.197 5.64e-05 ***
## tl_log               1.9836     0.3530   5.619 1.56e-07 ***
## locPetrohue         -2.3957     3.1494  -0.761    0.449
## locPuyehue          -2.0696     1.6868  -1.227    0.223
## tl_log:locPetrohue   0.4795     0.6928   0.692    0.490
## tl_log:locPuyehue    0.3624     0.3793   0.955    0.342
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3201 on 106 degrees of freedom
## Multiple R-squared:  0.8972, Adjusted R-squared:  0.8924
## F-statistic:   185 on 5 and 106 DF,  p-value: < 2.2e-16
```

Interpreting models with categorical X variables

Recall: Categorical X variables

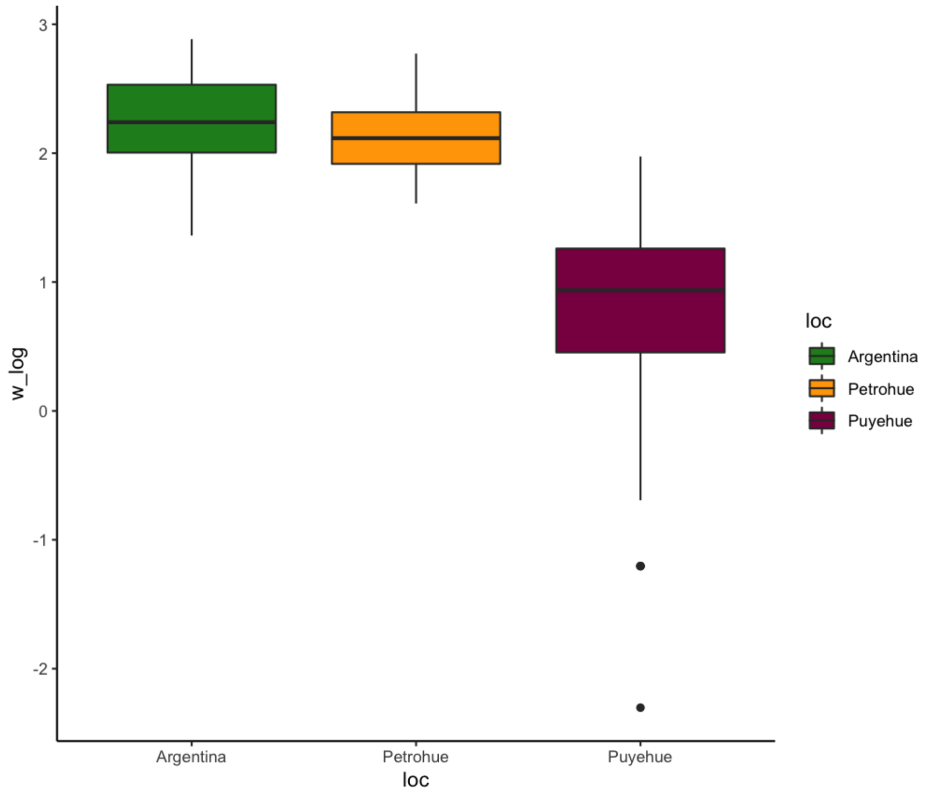
If X is categorical it doesn't make much sense to model $Y\ a + bX$ as X cannot be multiplied with b. But R has a workaround:

- categorical predictors are **converted into multiple continuous predictors**
- these are so-called **dummy variables**
- each dummy variable is coded as **0 (FALSE)** or **1 (TRUE)**
- the no. of dummy variables = no. of groups **minus 1**
- all linear models fit categorical predictors using dummy variables

Only categorical X

Differences of Chinook Salmon weight between three locations in Argentina

```
chin_mod <- lm(w_log ~ loc, ChinookArg)
```



Your turn...

How would you interpret these coefficients?

```r
chin_mod <- lm(w_log ~ loc, ChinookArg)
coef(chin_mod)
```

```
## (Intercept) locPetrohue  locPuyehue
##  2.25605528 -0.09844412 -1.52993775
```

What is the regression equation for each location?

How would you interpret these coefficients?

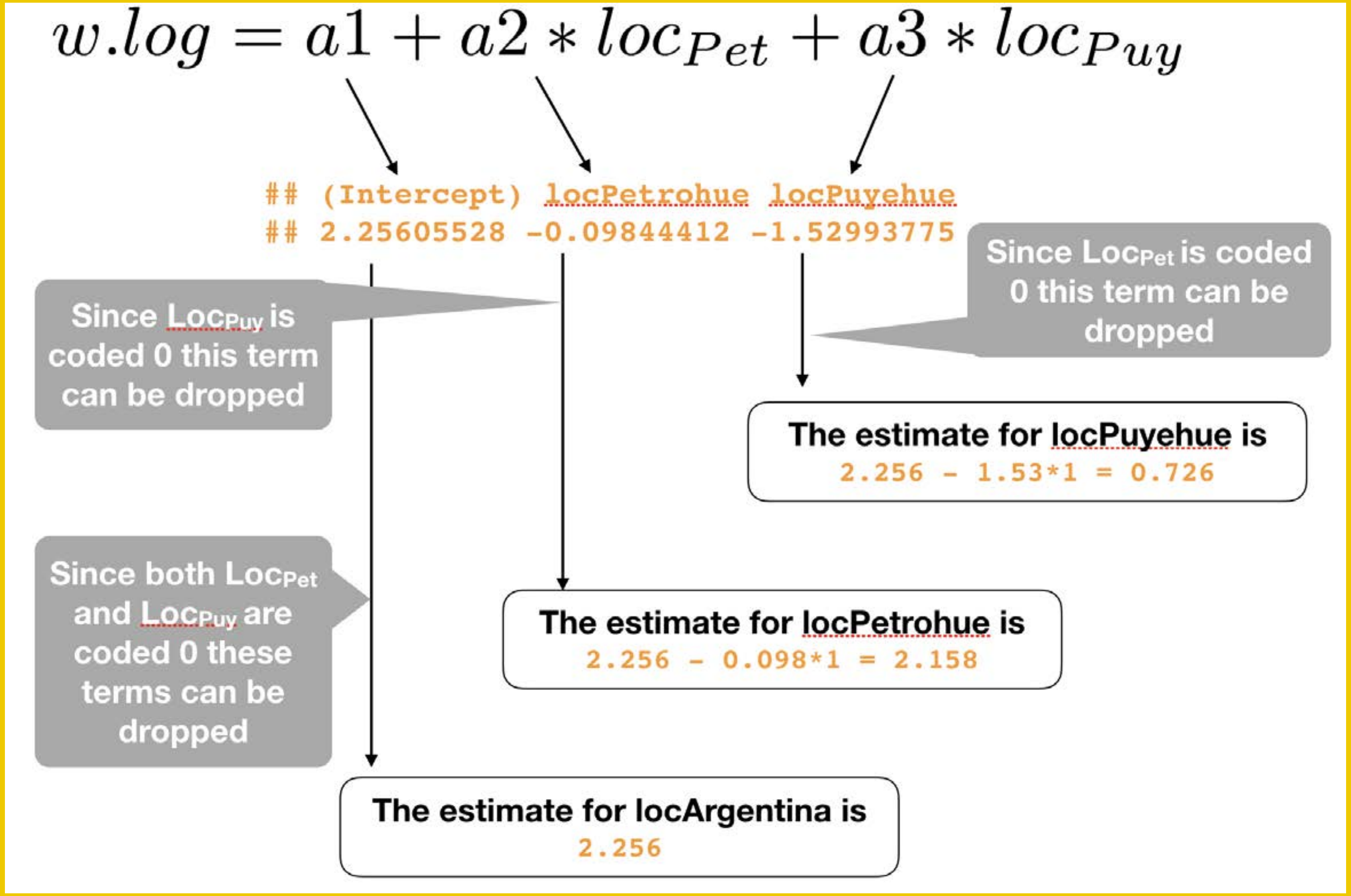
R generates dummy variable to be able to apply regressions on categorical variables. We can see this using the `model.matrix()` function:

```
model.matrix(w_log ~ loc, ChinookArg) %>%
    as.data.frame(.) %>%
  # adding the location variable from the original data
  mutate(sampl_loc = ChinookArg$loc) %>%
  head()
```

```
##   (Intercept) locPetrohue locPuyehue sampl_loc
## 1           1           0          0 Argentina
## 2           1           0          0 Argentina
## 3           1           0          0 Argentina
## 4           1           0          0 Argentina
## 5           1           0          0 Argentina
## 6           1           0          0 Argentina
```

We can see that the first 10 fish were sampled at the location 'Argentina' and that these observations were coded 1 for the variable 'intercept' (representing the first factor level → here Argentina) and 0 for the variable `locPetrohue` and `locPuyehue`.

Apply the estimated coefficients to the regression equation with dummy variables:


$w.log = a1 + a2 * loc_{Pet} + a3 * loc_{Puy}$
## (Intercept) locPetrohue locPuyehue
## 2.25605528 -0.09844412 -1.52993775
Since Loc_{Pet} is coded 0 this term can be dropped
Since Loc_{Puy} is coded 0 this term can be dropped
The estimate for locPuyehue is 2.256 - 1.53*1 = 0.726
Since both Loc_{Pet} and Loc_{Puy} are coded 0 these terms can be dropped
The estimate for locPetrohue is 2.256 - 0.098*1 = 2.158
The estimate for locArgentina is 2.256

Only categorical X - ANOVA

Linear regression with a categorical variable, is the equivalent of ANOVA (**ANalysis Of VAriance**). To see the output as an ANOVA table, use `anova()` on your lm object

```r
anova(chin_mod)
```

```
## Analysis of Variance Table
##
## Response: w_log
##            Df Sum Sq Mean Sq F value    Pr(>F)
## loc         2 60.542 30.2711  73.097 < 2.2e-16 ***
## Residuals 109 45.140  0.4141
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Only categorical X - ANOVA

Alternatively, use `aov()` instead of `lm()`

```
chin_aoc <- aov(w_log ~ loc, ChinookArg)
summary(chin_aoc)
```

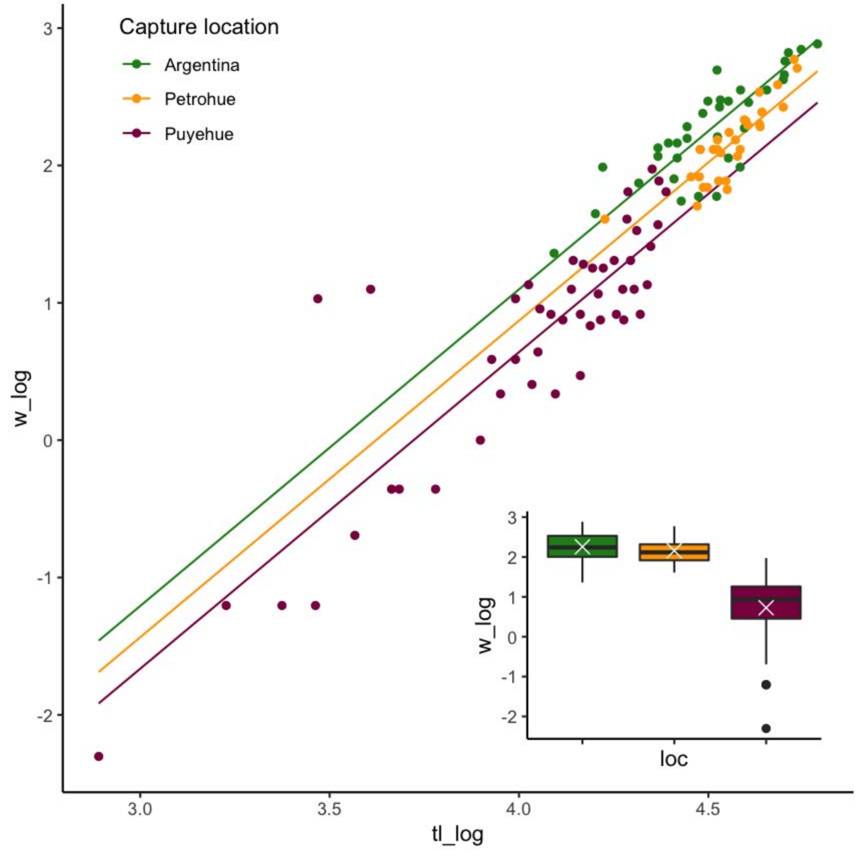
```
##              Df Sum Sq Mean Sq F value Pr(>F)    
## loc           2  60.54  30.271    73.1 <2e-16 ***
## Residuals   109  45.14   0.414                   
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Categorical and continuous X variables: ANCOVA

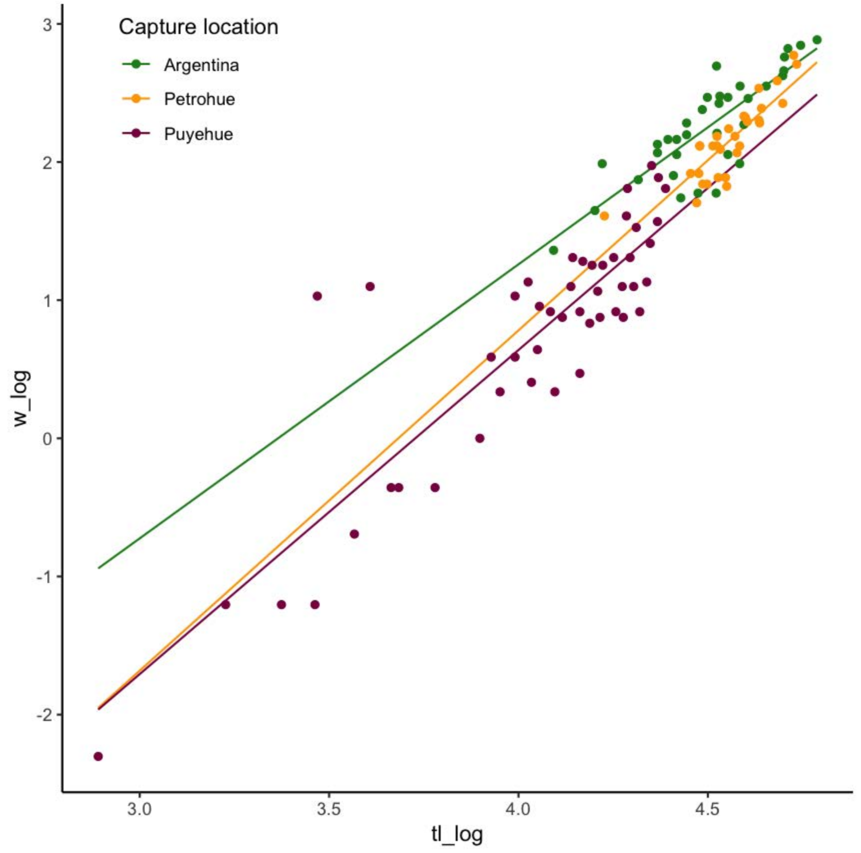
- **ANalysis of COVAriance** (ANCOVA) is a hybrid of a linear regression and ANOVA.
- Has at least one continuous and one categorical explanatory variable.
- Some consider ANCOVA as an "ANOVA"" model with a covariate included → focus on the factor levels adjusted for the covariate (e.g. Quinn & Keough 2002).
- Some consider it as a "Regression" model with a categorical predictor → focus on the covariate adjusted for the factor (e.g. Crawley 2007).
- The typical "maximal" model involves estimating an intercept and slope (regression part) for each level of the categorical variable(s) (ANOVA part) → i.e., including an interaction

Chinook Salmon weight as a function of location AND length

without interaction



with interaction



Regression view of an ANCOVA

$$w.log_{ij} = \alpha_i + \beta_i * tl.log_j + \epsilon_{ij}$$

where i = location, j = each individual fish

Regression view of an ANCOVA

Location-specific equations

$$w.log_{Arg,j} = \alpha_{Arg} + \beta_{Arg} * tl.log_j + \epsilon_{Arg,j}$$

$$w.log_{Pet,j} = \alpha_{Pet} + \beta_{Pet} * tl.log_j + \epsilon_{Pet,j}$$

$$w.log_{Puy,j} = \alpha_{Puy} + \beta_{Puy} * tl.log_j + \epsilon_{Puy,j}$$

Your turn...

ANCOVA Interpretation

Run the following 2 models and formulate for both models the location-specific equations with the estimated coefficients

```r
library(FSA)
ChinookArg <- mutate(ChinookArg,
  tl_log = log(tl), w_log = log(w))
chin_ancova1 <- lm(w_log ~ loc + tl_log, ChinookArg)
chin_ancova2 <- lm(w_log ~ loc * tl_log, ChinookArg)
```

Solution

ANCOVA 1 - no interaction

$$w.log = a1 + a2 * locPetrohue + a3 * locPuyehue + b * tl.log$$

The estimate for the mean weight at location *Argentina*:

$w.log_{Arg} = a1 + a2 * 0 + a3 * 0 + b * tl.log$= **-8.12+2.3*tl_log**

The estimate for the mean weight at location *Petrohue*:

$w.log_{Pet} = a1 + a2 * 1 + a3 * 0 + b * tl.log$

= -8.12+-0.23+2.3*tl_log = **-8.35 + 2.3*tl_log**

The estimate for the mean weight at location *Puyehue*:

$w.log_{Puy} = a1 + a2 * 0 + a3 * 1 + b * tl.log$

= -8.12+-0.46+2.3*tl_log = **-8.58+2.3 * tl_log**

ANCOVA 2 - with interaction

$$w.log = a1 + a2 * locPetrohue + a3 * locPuyehue + \\ b1 * tl.log + b2 * tl.log + b3 * tl.log$$

The estimate for the mean weight at location *Argentina*:

$w.log_{Arg}$ = **-6.67+2.3*tl_log**

The estimate for the mean weight at location *Petrohue*:

$w.log_{Pet}$ = -6.67+-2.4+1.98*tl_log+0.48*tl_log = **-9.07 + 2.46 * tl_log**

The estimate for the mean weight at location *Puyehue*:

$w.log_{Puy}$ = = -6.67+-2.07+1.98*tl_log+0.36*tl_log = **-8.74 + 2.34 * tl_log**

Statistical Modelling

Model selection

How to compare and choose the best model?

- Based on best goodness-of-fit: How well do the model fit a set of observations.
- How to judge this?
  - visually
  - using a criterion that summarize the discrepancy between observed values and the values expected under the model, e.g.
    - explained variance (R_2)
    - Akaike's Information Criterion (**AIC**) and modifications
    - Bayesian Information Criterion (**BIC**)
- A good book on that subject is written by Anderson & Burnham 2002: Model Selection and Multimodel Inference - A Practical Information-Theoretic Approach

Akaike's Information Criterion

$$AIC = \underbrace{N * \ln(SS_{Residual})}_{\text{measure of goodness of fit}} + \underbrace{2(p+1) - N * \ln(N)}_{\text{so-called penalty term for the number of independent parameters in the model}}$$

- The AIC is a **relative measure**, not an absolute as R^2: the values can only be compared between models **fitted to the same observations** and **same Y variables**. You can't compare models fitted to different data subsets or if Y is partly transformed!
- The lower the AIC the better.
- Rule of thumb: if difference between 2 models in AIC is **< 2** than choose the more simple model.
- R function: `AIC()`

Akaike's Information Criterion

Chinook example:

```r
m1 <- lm(w_log ~ loc, ChinookArg)
m2 <- lm(w_log ~ tl_log, ChinookArg)
m3 <- lm(w_log ~ loc + tl_log, ChinookArg)
m4 <- lm(w_log ~ loc * tl_log, ChinookArg)
AIC(m1, m2, m3, m4)
```

```
##    df       AIC
## m1  4 224.06339
## m2  3  87.69126
## m3  5  67.57480
## m4  7  70.53732
```

Which model shows the best performance based on the AIC?

Principle of parsimony (Occam‘s Razor):

- As few parameters as possible.
- Models should be minimal adequate.
- Simple explanations should be preferred.
- Linear models should be preferred to non-linear models.

Creationism is simpler than evolution. Applying Occam's Razor, creationism must be the right theory.
No, no! You're applying Occam's Razor all wrong. Let me show you how it's done.
Hey Occam! How's it going, dude? You look haggard.
Man, it's a nightmare. My roommates keep borrowing my razor.
Occam's Razor.
icanbarelydraw.com
CC BY-NC-ND 3.0

Beware

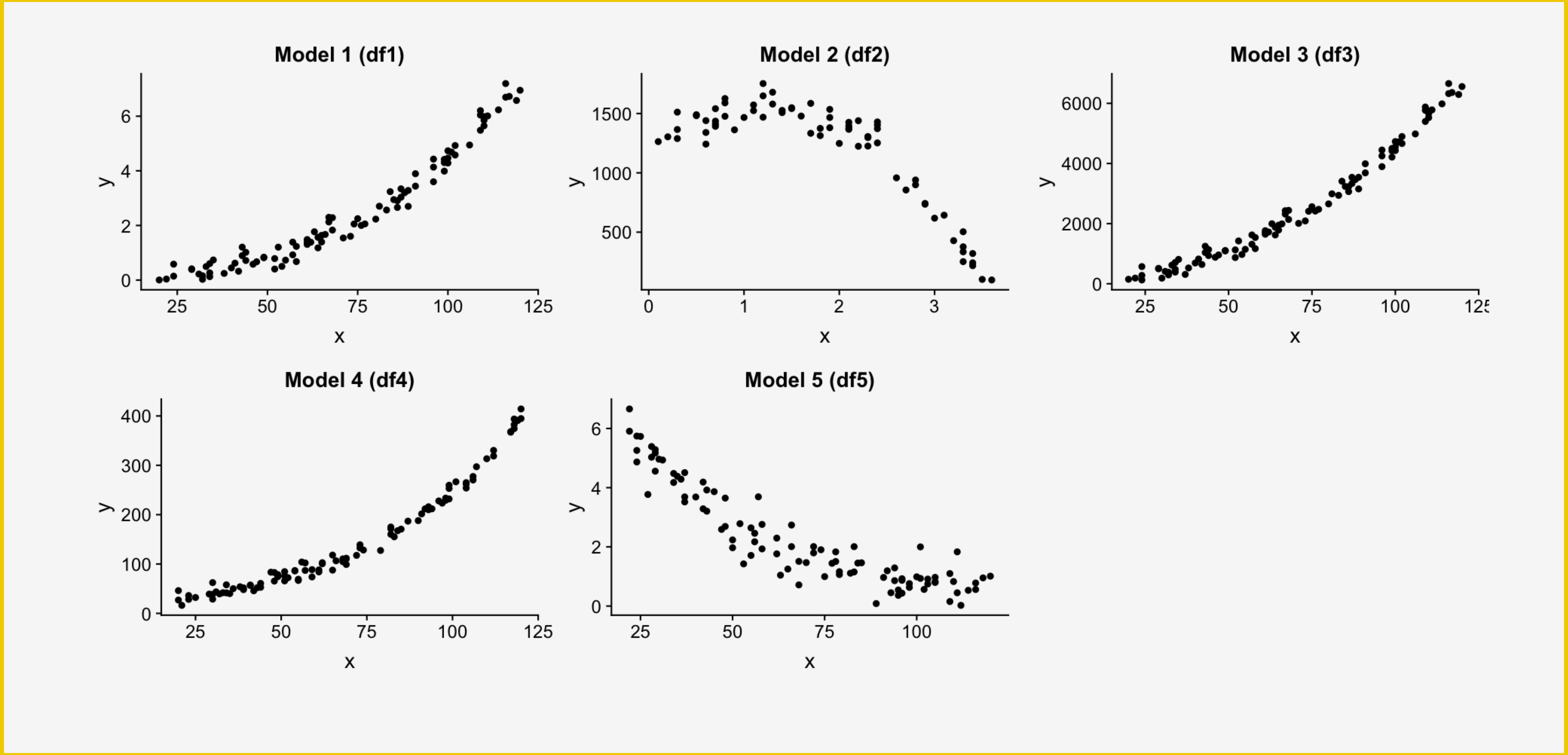
There is a temptation to become personally attached to a particular model. Statisticians call this 'falling in love with a model'.

Always keep in mind:

- All models are wrong, but some are useful.
- Some models are better than others.
- The correct model can never be known with certainty.
- The simpler the model, the better it is.

Your turn...

Exercise: Find the 'true' model or the underlying function



Exercise: Find the 'true' model or the underlying function

I generated different dataframes where the Y variable was modelled as a specific function of X plus some random noise. Load the datasets and see what objects you loaded with `ls()`

```
load("data/find_model.R")
ls()
```

You should see 10 dataframes. Try to find the 'true' models for df1, df2, df3, df4, and df5 by fitting different model families and compare their performance

- using the AIC (with function `AIC(model1, model2, model3,..)`) and
- plotting the predicted values to the observed ones and the residual histograms.

Once you think you found it, apply your models on the dataframes that do not contain the random noise (e.g. df1_nonoise for df1) and compare results.

Overview of functions for modelling and interpretation

WHAT	FUNCTION
Lin. regression & ANCOVA	`lm()`
ANOVA	`aov()` or `anova(lm())`
Coefficients	`coef(mod)`
Complete numerical output	`summary(mod)`
Confidence intervals	`confint(mod)`
Prediction	`predict(mod)`, `modelr::add_predictions(data, mod)`
Residuals	`resid(mod)`, `modelr::add_residuals(data, mod)`
Diagnostic plots	`plot(mod)`, `acf(resid(mod))`
Model comparison	`AIC(mod1, mod2, mod3)`

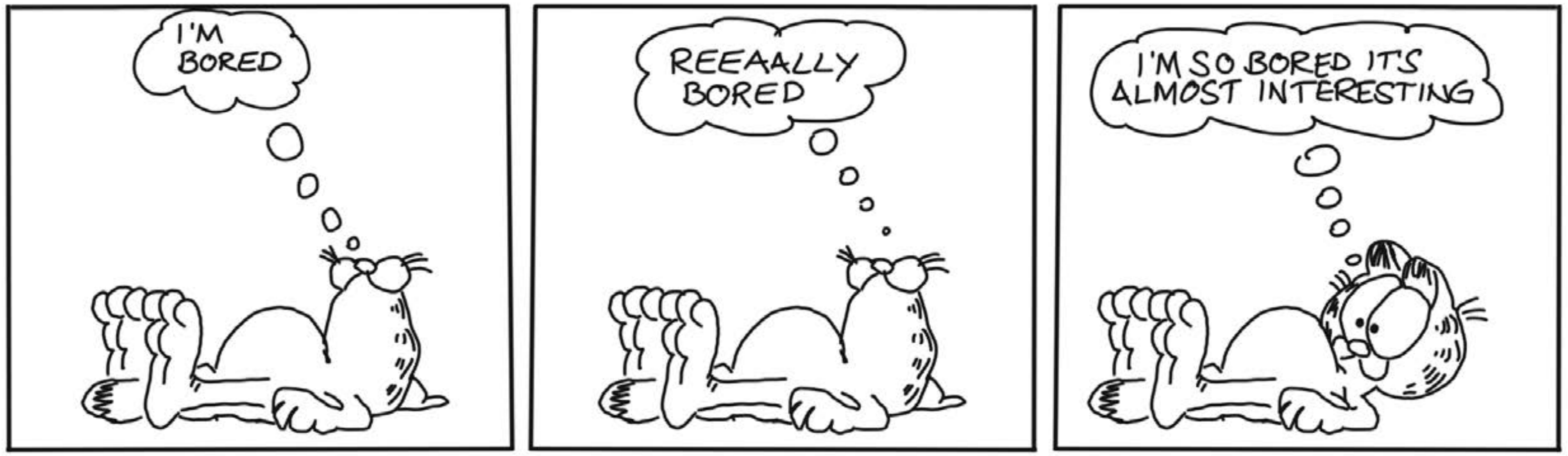
How do you feel now.....?

Totally confused?

Practice on the Chinook salmon dataset and read

- chapter 23 on model basics and chapter 24 on model building in the "R for Data Science"" book, as well as
- chapter 9 (statistical modelling) in "The R book" (Crawley, 2013) (an online pdf version is freely available here).

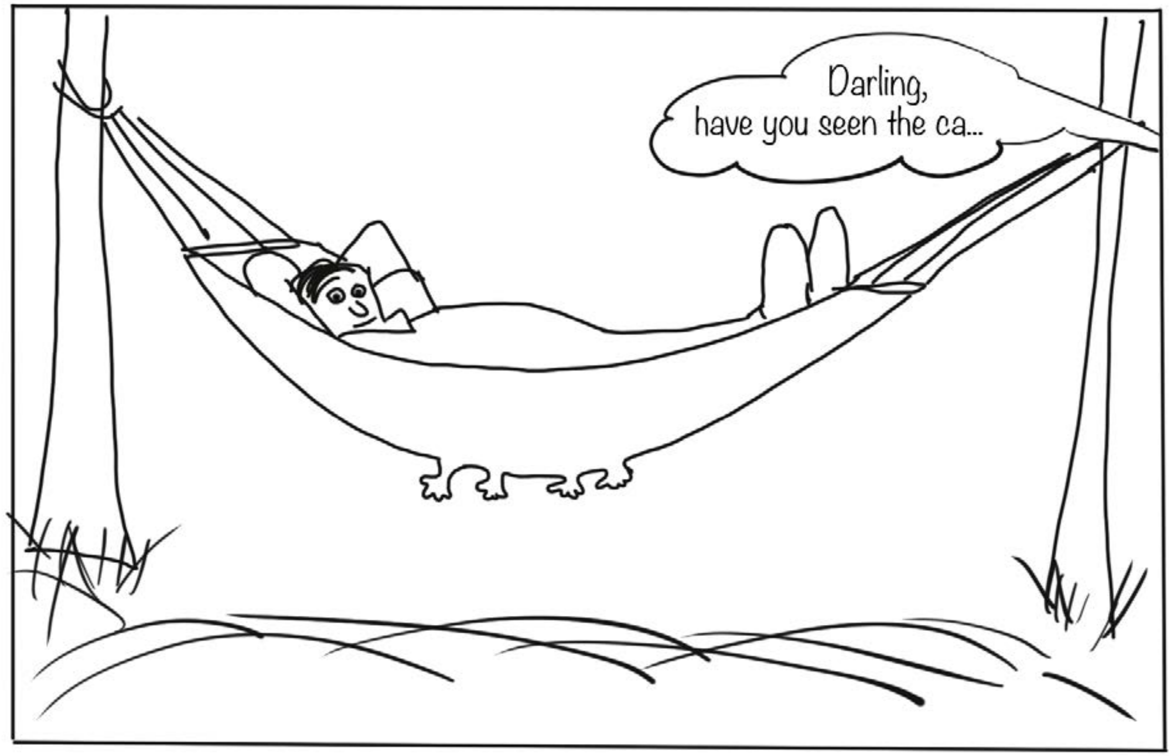
Totally bored?



Stay tuned for the next case study where you can play around as much as you want to!

Totally content?

Then go grab a coffee, lean back and enjoy the rest of the day...!



Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

Thank You

For more information contact me: saskia.otto@uni-hamburg.de

http://www.researchgate.net/profile/Saskia_Otto
http://www.github.com/saskiaotto

Solution

Example to find the best model: `df1`

1.Apply different models and compare first their AIC.

```r
load("data/find_model.R")
dat <- df1 # this way you can simply
# replace the dataframes later
dat$y_log <- log(dat$y + 0.001)
dat$x_log <- log(dat$x)

m1 <- lm(y ~ x, data = dat)
m2 <- lm(y ~ poly(x,2), data = dat)
m3 <- lm(y ~ poly(x,3), data = dat)
m4 <- lm(y_log ~ x, data = dat)
m5 <- lm(y_log ~ x_log, data = dat)
```

```r
AIC(m1,m2,m3)
```

```
##    df       AIC
## m1  3 185.24425
## m2  4  37.56960
## m3  5  34.61143
```

```r
AIC(m4,m5)
```

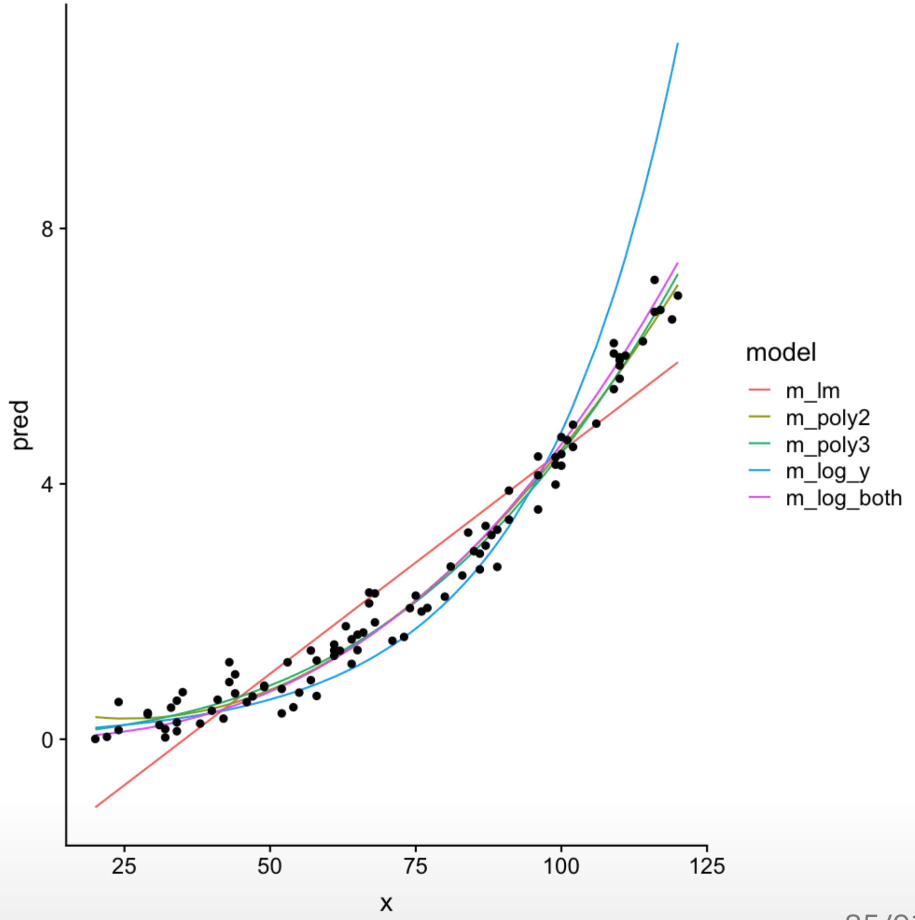
```
##    df      AIC
## m4  3 174.5666
## m5  3 139.7156
```

Note:
The AIC can only be compared between models that are fitted on the same datasets! Hence, models with log-transformed Y values and those without CANNOT be compared using the AIC.

Example to find the best model: `df1`

2.Prediction plots → to compare all models at the same scale, back-transform the log-model predictions

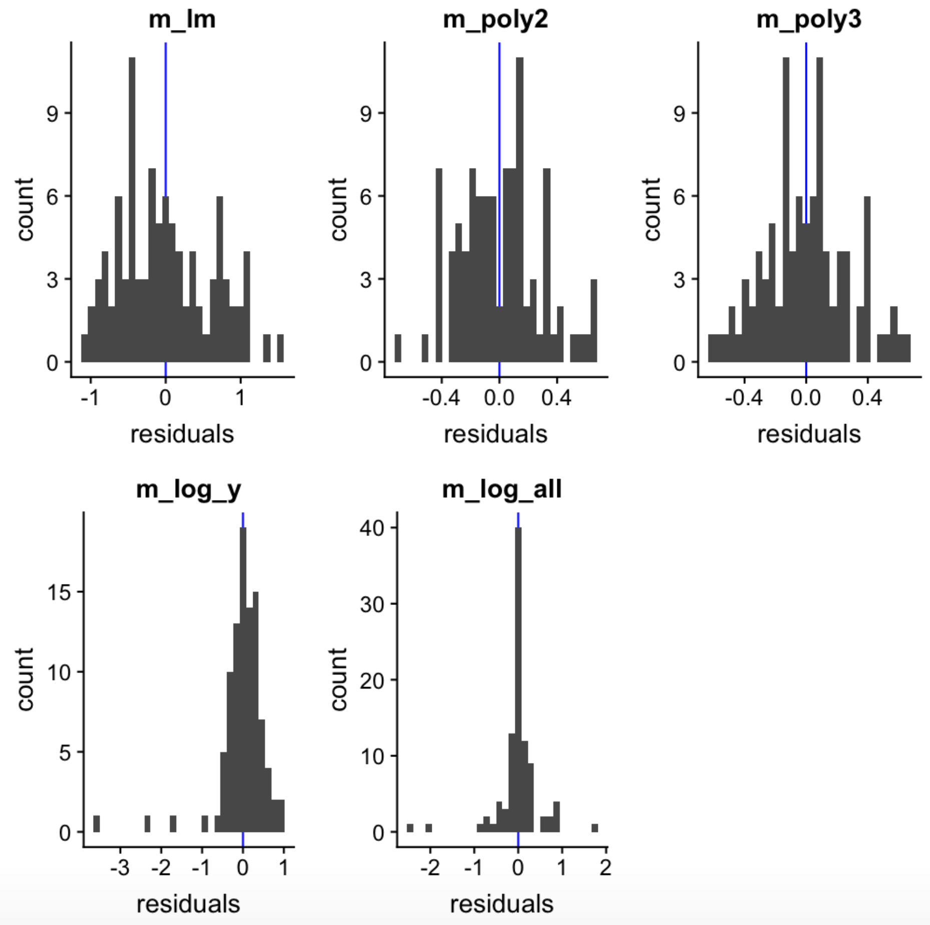
```
dat <- spread_predictions(
    data = dat, m1,m2,m3,m4,m5) %>%
  mutate(m4 = (exp(m4) - 0.001),
    m5 = (exp(m5) - 0.001))

dat_long <- dat %>%
  select(x, m1,m2,m3,m4,m5) %>%
  gather(key = "model", "pred", -x) %>%
  mutate(model = factor(model,
    labels = c("m_lm", "m_poly2",
    "m_poly3","m_log_y","m_log_both")))

dat_long %>% ggplot(aes(x,pred)) +
  geom_line(aes(colour = model)) +
  geom_point(data = dat, aes(y = y))
```



Example to find the best model: `df1`

3.Residual plots

```r
# Residual plots
r <- dat %>%
  spread_residuals(m1,m2,m3,m4,m5) %>%
  ggplot()+ geom_vline(xintercept = 0,
    colour = "blue", size = 0.5)
r1 <- r + ggtitle("m_lm") +
  geom_histogram(aes(x = m1)) +
r2 <- r + ggtitle("m_poly2") +
  geom_histogram(aes(x = m2))
r3 <- r + ggtitle("m_poly3") +
  geom_histogram(aes(x = m3))
r4 <- r + ggtitle("m_log_y") +
  geom_histogram(aes(x = m4))
r5 <-  r + ggtitle("m_log_all") +
  geom_histogram(aes(x = m5))
gridExtra::grid.arrange(grobs =
list(r1,r2,r3,r4,r5), ncol = 3)
```



Example to find the best model: `df1`

The AIC indicates best performances for models **m3** (polynomial of order 3) and **m5** (X and X both log-transformed). Also the prediction plots and the residual plots support this. In fact, the prediction plot does not show a big difference between both models. The residual plots, on the other hand, might provide some support for m5 as a high number of y values deviate little from their predictions.

To really find out which model has the true underlying function, used to create this dataset, we need to apply the models on the dataset without noise:

Example to find the best model: `df1_nonoise`

1.Apply models to the data without noise

```r
dat <- df1_nonoise
dat$y_log <- log(dat$y + 0.001)
dat$x_log <- log(dat$x)

m1 <- lm(y ~ x, data = dat)
m2 <- lm(y ~ poly(x,2), data = dat)
m3 <- lm(y ~ poly(x,3), data = dat)
m4 <- lm(y_log ~ x, data = dat)
m5 <- lm(y_log ~ x_log, data = dat)
```

```r
AIC(m1,m2,m3)
```

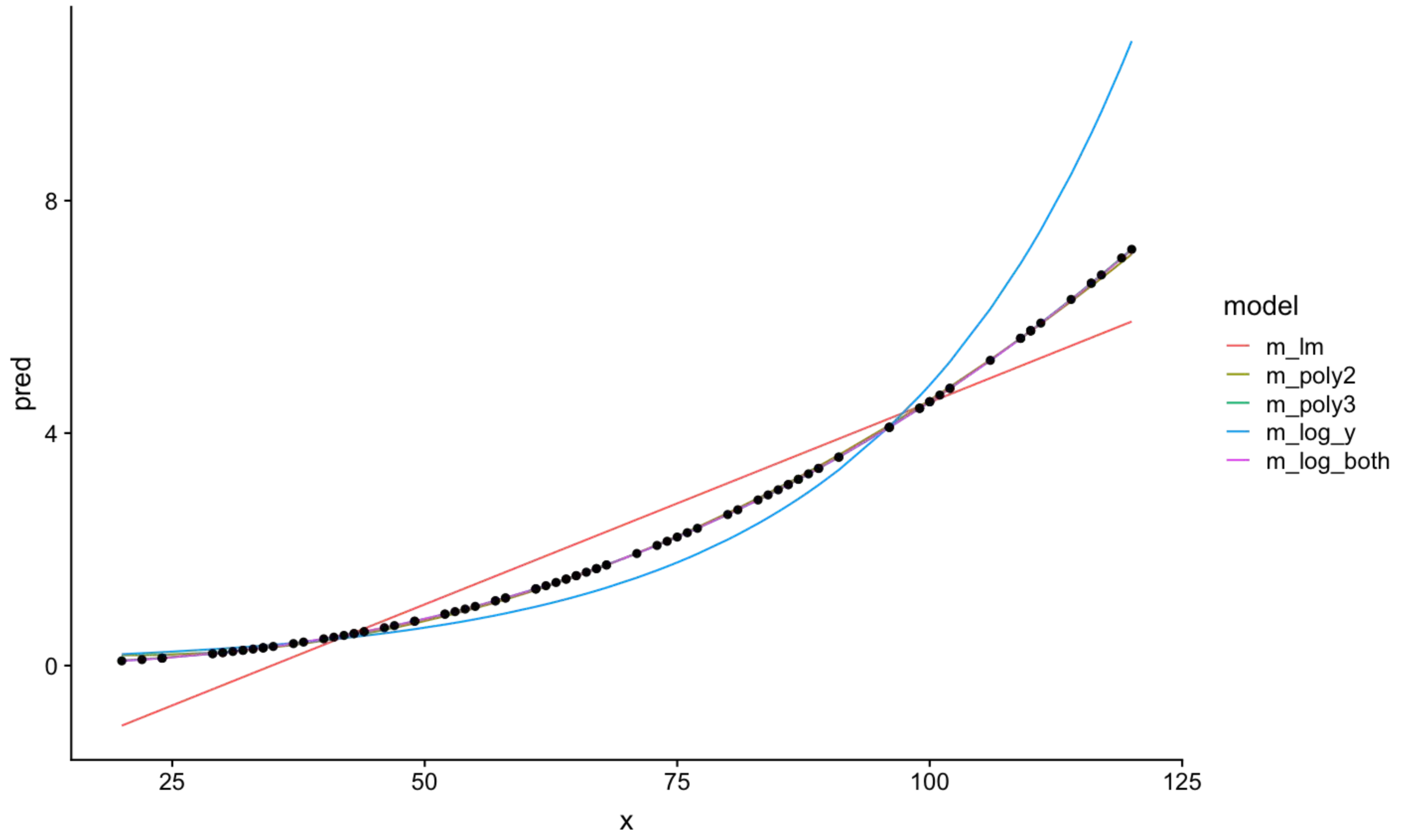
```
##    df       AIC
## m1  3  156.3179
## m2  4 -397.3983
## m3  5 -990.3074
```

```r
AIC(m4,m5)
```

```
##    df         AIC
## m4  3    11.89622
## m5  3 -1066.44843
```

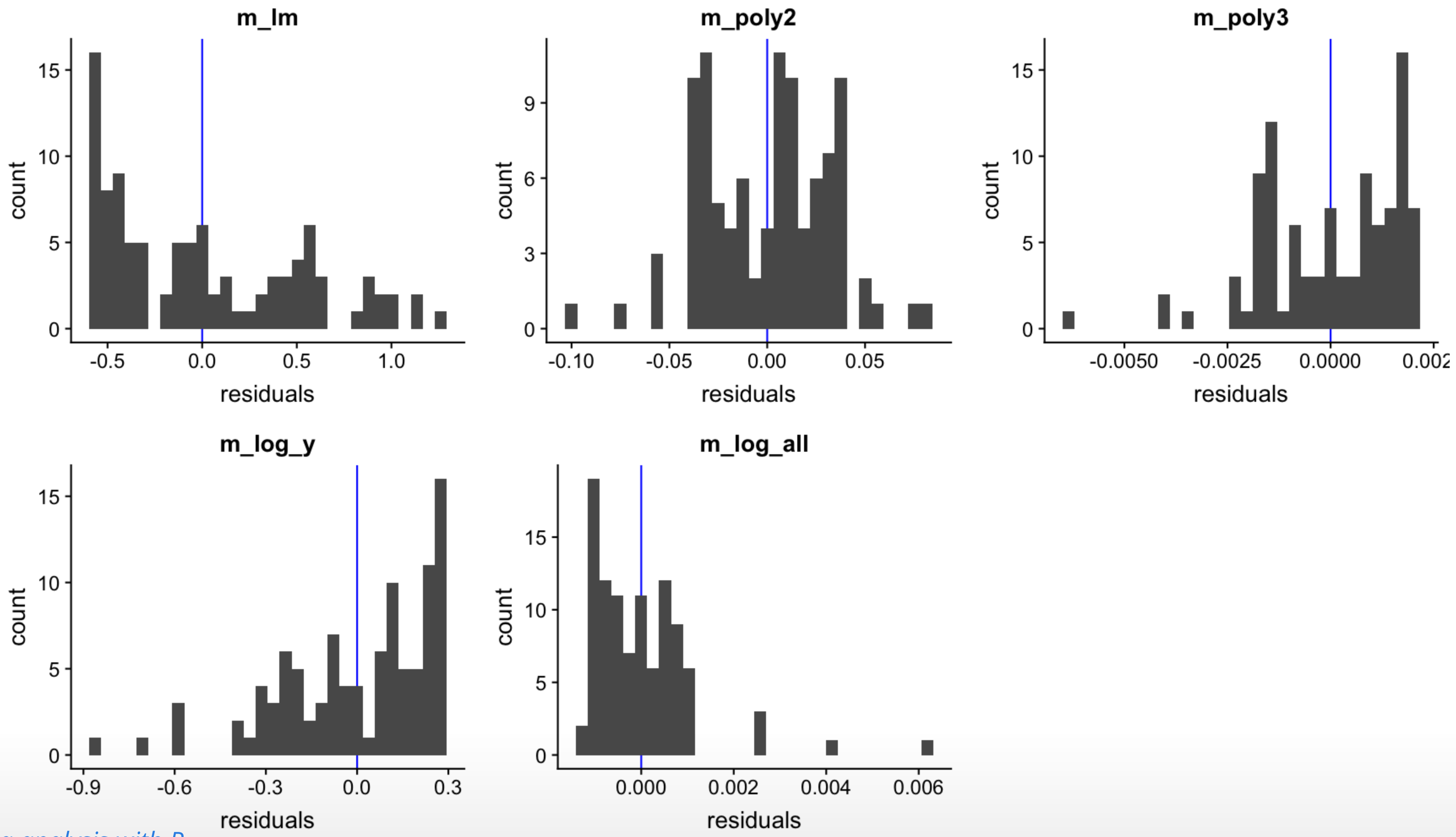
Example to find the best model: `df1_nonoise`

2.Prediction plots without noise



Example to find the best model: `df1_nonoise`

3.Residual plots without noise



Example to find the best model: `df1_nonoise`

Now it becomes clear that the underlying function is an exponental function of the form $Y = aX^b$.

For comparison:

```r
# This is the true underlying function
set.seed(123)
x <- sample(20:120, size = 100,
  replace = TRUE)
y_noise <- rnorm(100, 0, 0.3)
a <- exp(-10)
b <- 2.5
y <- a * x^b + y_noise
```

```r
m5_comp <- lm(log(y) ~ log(x))
coefficients(m5_comp)
```

```
## (Intercept)      log(x)
##  -10.662521    2.648546
```

Solution of all 5 models

df1: $Y_i = aX_i^b + \epsilon_i$, with a = exp(-10), b = 2.5

df2: $Y_i = a + b1X_i + b2X_i^2 + b3X_i^3 + \epsilon_i$, with a = 1250, b1 = 400, b2 = -100, b3 = -30

df3: $Y_i = a + b1X_i + b2X_i^2 + \epsilon_i$, with a = 100, b1 = -5, b2 = 0.5

df4: $Y_i = ae^{bX_i} + \epsilon_i$, with a = 20, b = 0.025

df5: $Y_i = ae^{-bX_i} + \epsilon_i$, with a = 10, b = -0.025