Solution 1: HRO in `mlr3`

a) Model classes representing a certain **hypothesis** are stored in `learner` objects. Before training them on actual data, they just contain information on the functional form of f. Once a learner has been trained we can examine the parameters of the resulting model. The empirical **risk** can be assessed after training by several performance measures (e.g., based on $L2$ loss). **Optimization** happens rather implicitly as `mlr3` only acts as a wrapper for existing implementations and calls package-specific optimization procedures.

b)
```
library(mlr3)
mlr3::tsk("iris")

## <TaskClassif:iris> (150 x 5): Iris Flowers
## * Target: Species
## * Properties: multiclass
## * Features (4):
##   - dbl (4): Petal.Length, Petal.Width, Sepal.Length, Sepal.Width
```

We obtain the following information:

- `iris` is a classification task.
- It has 150 observations of 5 variables, one of which is the target.
- The target `Species` contains more than 2 classes.
- We have 4 features, all of them floating numbers (`dbl`).

If necessary, we can specify further task attributes. For example, we might have one feature that merely stores unique identifiers for each observation. `mlr3` allows us to set the *role* of this variable to an ID variable. We can also assign roles of weighting or stratifying variables in analogous fashion. Other task attributes include the number of missing values per feature and the so-called *backend* (the raw data we created our task from – besides using predefined tasks like `iris` it is possible to specify tasks from any data of suitable format).

c) Let's have a look at the available learners (in case you are wondering why this list is so short: there is a dedicated extension package, `mlr3learners`, that holds other learners besides these most basic ones, and there is even `mlr3extralearners`):

```
mlr3::mlr_learners$keys()

## [1] "classif.debug"       "classif.featureless" "classif.rpart"
## [4] "regr.debug"          "regr.featureless"    "regr.rpart"
```

Let's check out the **regression tree** learner. Roughly speaking, regression trees create small, homogeneous subsets ("nodes") by repeatedly splitting the data at some cut-off (e.g., for `iris`: partition into observations with `Sepal.Width` ≤ 3 and > 3), and predict the mean target value within each final group.

```
mlr3::lrn("regr.rpart")

## <LearnerRegrRpart:regr.rpart>: Regression Tree
## * Model: -
## * Parameters: xval=0
## * Packages: mlr3, rpart
## * Predict Types:  [response]
## * Feature Types: logical, integer, numeric, factor, ordered
## * Properties: importance, missings, selected_features, weights
```

We obtain the following information:

- `regr.rpart` is a *regression* learner (as you may have noticed above, there is a separate tree learner for classification).
- It has not been trained yet, so no model is stored.
- The underlying package is `rpart`.
- `regr.rpart` predicts *response* (unsurprisingly, but classification learners might also predict *probabilities*).
- It supports boolean, numerical and categorical features (but no date variables, for instance).
- Special properties include the ability to handle missing values and compute feature importance.
- Regarding hyperparameters, we see that some `xval` has been set (the function reference can be found at `https://cran.r-project.org/web/packages/rpart/rpart.pdf`). However, there is typically a whole bunch of configurable hyperparameters:

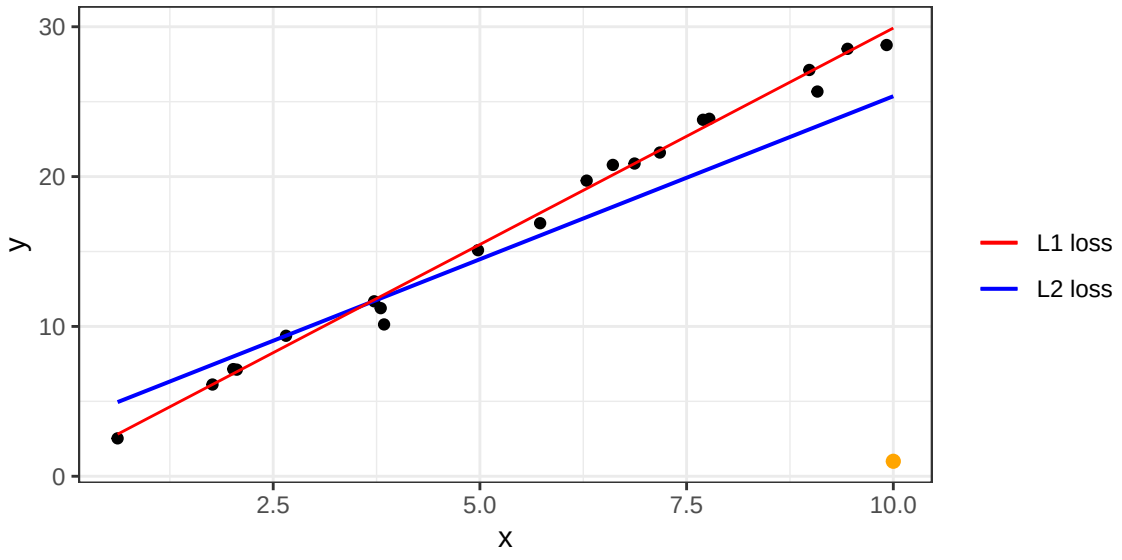
```
mlr3::lrn("regr.rpart")$param_set
```

```
## <ParamSet>
##                id    class lower upper nlevels        default value
##  1:             cp ParamDbl     0     1     Inf           0.01
##  2:     keep_model ParamLgl    NA    NA       2          FALSE
##  3:     maxcompete ParamInt     0   Inf     Inf              4
##  4:       maxdepth ParamInt     1    30      30             30
##  5:   maxsurrogate ParamInt     0   Inf     Inf              5
##  6:      minbucket ParamInt     1   Inf     Inf <NoDefault[3]>
##  7:       minsplit ParamInt     1   Inf     Inf             20
##  8: surrogatestyle ParamInt     0     1       2              0
##  9:   usesurrogate ParamInt     0     2       3              2
## 10:           xval ParamInt     0   Inf     Inf             10     0
```

We might, for example, override the default of `minsplit`, which states the minimum number of observations a node must contain to be split further.

Solution 2: Loss Functions for Regression Tasks

a) $L2$ loss penalizes vertical distances to the regression line *quadratically*, while $L1$ only considers the *absolute* distance. As the outlier point lies pretty far from the remaining training data, it will have a large loss with $L2$, and the regression line will pivot to the bottom right to minimize the resulting empirical risk. A model trained with $L1$ loss is less susceptible to the outlier and will adjust only slightly to the new data.



b) The Huber loss combines the respective advantages of $L1$ and $L2$ loss: it is smooth and (once) differentiable like $L2$ but does not punish larger residuals as severely, leading to more robustness. It is simply a (weighted) piecewise combination of both losses, where ϵ marks where $L2$ transits to $L1$ loss. The exact definition is:

$$L\left(y, f(\mathbf{x})\right) = \begin{cases} \frac{1}{2}(y - f(\mathbf{x}))^2 & \text{if } |y - f(\mathbf{x})| \leq \epsilon \\ \epsilon|y - f(\mathbf{x})| - \frac{1}{2}\epsilon^2 & \text{otherwise} \end{cases}, \quad \epsilon > 0$$

In the plot we can see how the parabolic shape of the loss around 0 evolves into an absolute-value function at $|y - f(\mathbf{x})| > \epsilon = 5$.

c) We solve this just like any other optimization problem: setting the derivative to 0 and solving for $\boldsymbol{\theta}$.

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 &= 0 \\ \frac{\partial}{\partial \boldsymbol{\theta}} \left((\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \right) &= 0 \\ \frac{\partial}{\partial \boldsymbol{\theta}} \left(\mathbf{y}^\top \mathbf{y} - 2\boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{y} + \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} \right) &= 0 \\ -2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} &= 0 \\ \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} &= \mathbf{X}^\top \mathbf{y} \\ \hat{\boldsymbol{\theta}} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \end{aligned}$$

Don't be spooked by the matrix notation – just make sure you know basic linear algebra, e.g.,

$$(\mathbf{AB})^\top = \mathbf{B}^\top \mathbf{A}^\top,$$

and remind yourself of the analogies between scalar and matrix-valued calculations (e.g., x^2 translates to $\mathbf{X}^\top \mathbf{X}$, and $\frac{1}{x}$ to $\mathbf{X}^{-1}$). As this is a tool you will need to handle frequently, refresh your algebra if necessary.

A good reference in general is "Mathematics for Machine Learning" by Deisenroth et al. (for the above, you might want to have a look at *vector calculus*), freely available at `https://mml-book.github.io/book/mml-book.pdf`.

Solution 3: Polynomial Regression

a) *Cubic* means degree 3, so our hypothesis space will look as follows:

$$\mathcal{H} = \{f(\mathbf{x} \mid \boldsymbol{\theta}) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 \mid (\theta_0, \theta_1, \theta_2, \theta_3)^\top \in \mathbb{R}^4\}$$

b) Choose 3 different parameterizations and plot the resulting polynomials:

```
library(ggplot2)

# Simulate data
set.seed(123L)
x <- seq(-3, 3, length.out = 50)
y <- -3 + 5 * sin(0.4 * pi * x) + rnorm(50, sd = 1)
data <- data.frame(x, y)

# Generate design matrix by taking x to the power of 0 through 3
X <- as.matrix(sapply(0:3, function(i) x^i))
head(X)

##      [,1]      [,2]     [,3]      [,4]
## [1,]    1 -3.000000 9.000000 -27.00000
## [2,]    1 -2.877551 8.280300 -23.82699
```

```
## [3,]    1 -2.755102 7.590587 -20.91284
## [4,]    1 -2.632653 6.930862 -18.24656
## [5,]    1 -2.510204 6.301125 -15.81711
## [6,]    1 -2.387755 5.701374 -13.61349
```

```
# Define 3 different values for each theta_j
thetas <- matrix(cbind(
  c(-3, 1, 1.5),
  c(5, -1.6, 2),
  c(0, -0.3, -0.7),
  c(-0.8, 0.2, 0)),
  ncol = 4)
thetas
```

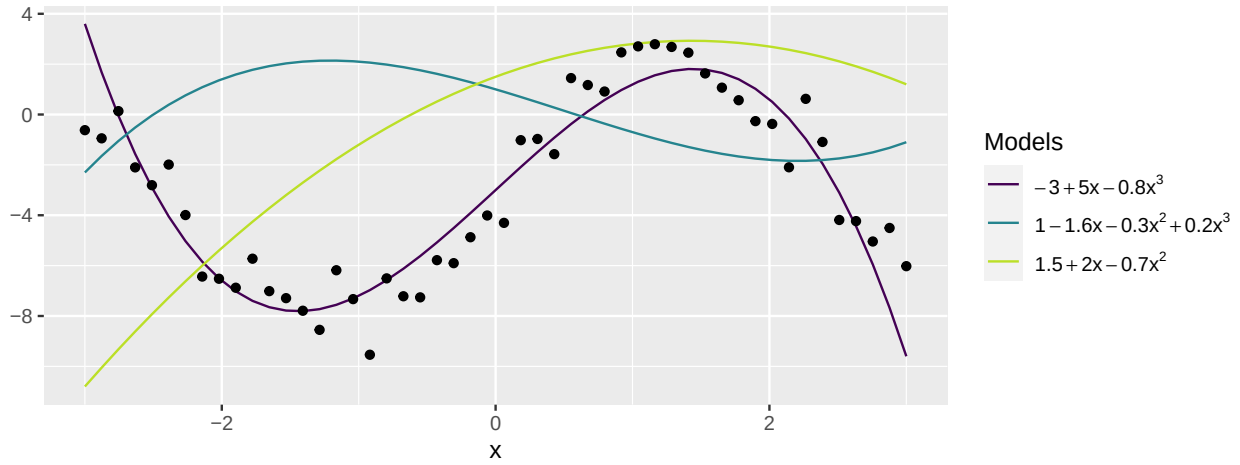
```
##      [,1] [,2] [,3] [,4]
## [1,] -3.0  5.0  0.0 -0.8
## [2,]  1.0 -1.6 -0.3  0.2
## [3,]  1.5  2.0 -0.7  0.0
```

```
# Compute the resulting models
f_hat <- sapply(1:3, function(i) X %*% thetas[i, ])
data_models <- data.frame(x, f_hat)
names(data_models) <- c("x", sprintf("f_hat_%i", 1:3))
head(data_models)
```

```
##           x     f_hat_1     f_hat_2    f_hat_3
## 1 -3.000000  3.60000000 -2.30000000 -10.800000
## 2 -2.877551  1.67383318 -1.64540540 -10.051312
## 3 -2.755102 -0.04523625 -1.05158140  -9.323615
## 4 -2.632653 -1.56602096 -0.51632483  -8.616910
## 5 -2.510204 -2.89733359 -0.03743253  -7.931195
## 6 -2.387755 -4.04798681  0.38729866  -7.266472
```

```
# Convert data to long format
data_models_long <- reshape2::melt(
  data_models,
  id.vars = "x",
  measure.vars = c("f_hat_1", "f_hat_2", "f_hat_3"))
```

```
# Plot the corresponding polynomial functions
ggplot2::ggplot(data_models_long, aes(x = x, y = value, col = variable)) +
  ggplot2::geom_line() +
  ggplot2::scale_color_viridis_d(
    "Models",
    end = 0.9,
    labels = c(
      bquote(-3 + 5 * x - 0.8 * x**3),
      bquote(1 - 1.6 * x - 0.3 * x**2 + 0.2 * x**3),
      bquote(1.5 + 2 * x - 0.7 * x**2))) +
  ggplot2::geom_point(data, mapping = aes(x, y), inherit.aes = FALSE) +
  ggplot2::ylab("")
```



We see that our hypothesis space is simply a family of curves. The 3 examples plotted here already hint at the amount of flexibility third-degree polynomials offer over simple linear functions.

c) The empirical risk is:

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{50} \left(y^{(i)} - \left[\theta_0 + \theta_1 x^{(i)} + \theta_2 \left(x^{(i)} \right)^2 + \theta_3 \left(x^{(i)} \right)^3 \right] \right)^2$$

d) Denoting our transformed feature matrix by $\tilde{\mathbf{X}}$, we can find the gradient just as we did for an intermediate result when we derived the least-squares estimator:

$$\begin{aligned} \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) &= \frac{\partial}{\partial \boldsymbol{\theta}} \left\| \mathbf{y} - \tilde{\mathbf{X}}\boldsymbol{\theta} \right\|_2^2 \\ &= \frac{\partial}{\partial \boldsymbol{\theta}} \left(\left(\mathbf{y} - \tilde{\mathbf{X}}\boldsymbol{\theta} \right)^\top \left(\mathbf{y} - \tilde{\mathbf{X}}\boldsymbol{\theta} \right) \right) \\ &= -2\tilde{\mathbf{X}}^\top \mathbf{y} + 2\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\boldsymbol{\theta} \\ &= 2 \cdot \left(-\tilde{\mathbf{X}}^\top \mathbf{y} + \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\boldsymbol{\theta} \right) \end{aligned}$$

e) Recall that the idea of gradient descent (*descent*!) is to traverse the risk surface in the direction of the *negative* gradient as we are in search for the minimum. Therefore, we will update our current parameter set $\boldsymbol{\theta}^{[t]}$ with the negative gradient of the current empirical risk w.r.t. $\boldsymbol{\theta}$, scaled by learning rate (or step size) α:

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha \cdot \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[t]}).$$

Note that the $L2$-induced multiplicative constant of 2 in the gradient can simply be absorbed by $\tilde{\alpha} := \frac{1}{2}\alpha$:

$$\underbrace{\boldsymbol{\theta}^{[t+1]}}_{p\times 1} = \underbrace{\boldsymbol{\theta}^{[t]}}_{p\times 1} - \tilde{\alpha} \cdot \left(- \underbrace{\tilde{\mathbf{X}}^\top}_{p\times n} \underbrace{\mathbf{y}}_{n\times 1} + \underbrace{\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}}_{p\times p} \underbrace{\boldsymbol{\theta}^{[t]}}_{p\times 1} \right)$$

$$\begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{pmatrix}^{[t+1]} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{pmatrix}^{[t]} - \tilde{\alpha} \cdot \left(-\tilde{\mathbf{X}}^\top \mathbf{y} + \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{pmatrix}^{[t]} \right)$$

What actually happens here: we update each component of our current parameter vector $\boldsymbol{\theta}^{[t]}$ in the *direction* of the negative gradient, i.e., following the steepest downward slope, and also by an *amount* that depends on the value of the gradient.

In order to see what that means it is helpful to recall that the gradient $\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ tells us about the effect (infinitesimally small) changes in $\boldsymbol{\theta}$ have on $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$. A parameter vector component with large gradient has strong impact on the empirical risk, and it is reasonable to assume it to be rather important for the model.

Therefore, gradient updates focus on influential components, and we proceed more quickly along the important dimensions.

f) We see that, for example, the first model in exercise b) fits the data fairly well but not perfectly. Choosing a more flexible function (a polynomial of higher degree or a function from an entirely different, more complex, model class) might be advantageous:

- We would be able to trace the observations more closely if our function were less smooth, and thus reduce empirical risk.
- Also, we might achieve a better fit on the boundaries of the input space where the cubic polynomials diverge pretty quickly.

On the other hand, flexibility also has some drawbacks:

- Flexible model classes often have more parameters, making training harder.
- We might run into a phenomenon called **overfitting**. Recall that our ultimate goal is to make predictions on *new* observations (after all, we know the labels for the training data). However, fitting every quirk of the training observations – possibly caused by imprecise measurement or other factors of randomness/error – will not generalize so well to new data.

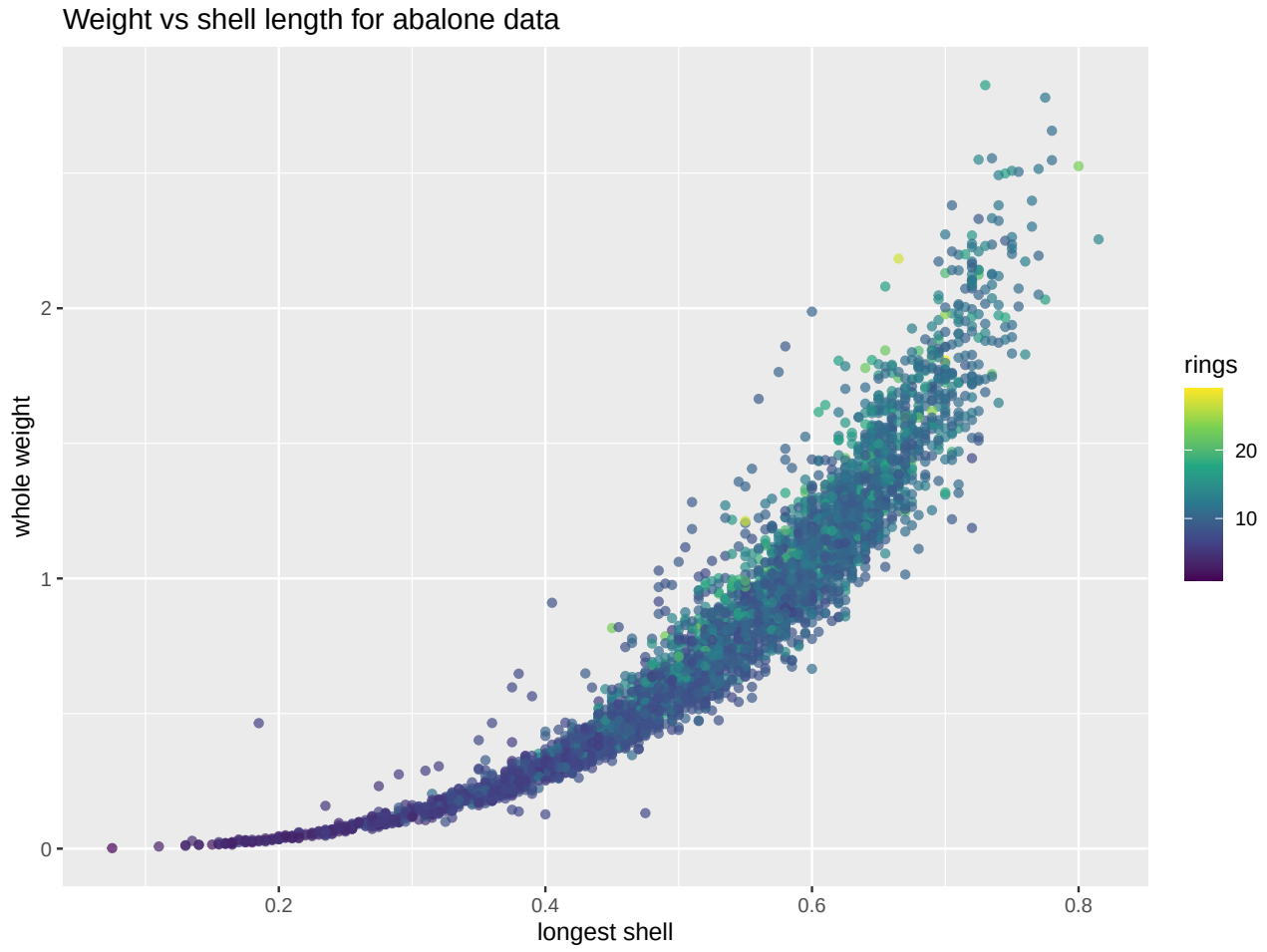
In the end, we need to balance model fit and generalization. We will discuss the choice of hypotheses quite a lot since it is one of the most crucial design decisions in machine learning.

Solution 4: Predicting `abalone`

Preparation:

```r
# Download data
url <- "https://archive.ics.uci.edu/ml/machine-learning-databases/abalone/abalone.data"
abalone <- read.table(url, sep = ",", row.names = NULL)
colnames(abalone) <- c(
  "sex", "longest_shell", "diameter", "height", "whole_weight",
  "shucked_weight", "visceral_weight", "shell_weight", "rings")

# Reduce to relevant columns
abalone <- abalone[, c("longest_shell", "whole_weight", "rings")]

# Reduce to relevant columns
abalone <- abalone[, c("longest_shell", "whole_weight", "rings")]
```

a)
```r
library(ggplot2)

# Plot weight vs shell length
ggplot2::ggplot(
  abalone,
  aes(x = longest_shell, y = whole_weight, col = rings)) +
  ggplot2::geom_point(alpha = 0.7) +
  ggplot2::scale_color_viridis_c() +
  ggplot2::labs(
    x = "longest shell",
    y = "whole weight",
    title = "Weight vs shell length for abalone data")
```



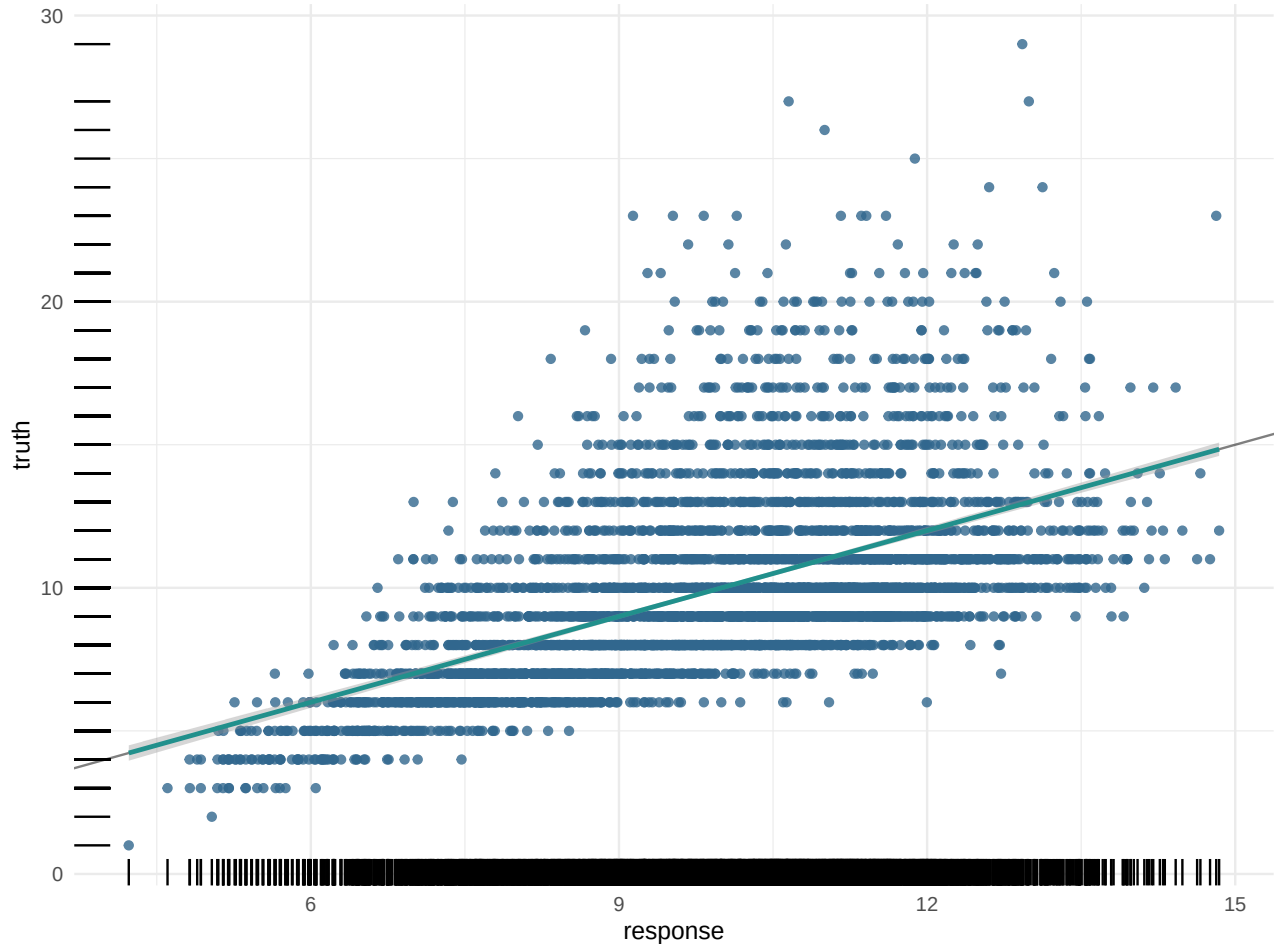
We see that weight scales exponentially with shell length and that larger/heavier animals tend to have more rings.

b)
```
library(mlr3)

# Specify regression task
task_abalone <- mlr3::TaskRegr$new(
  id = "abalone", backend = abalone, target = "rings")
```

c)
```
library(mlr3learners)

# Set up LM, train (by default, the target will be regressed on all features,
# i.e., target ~ .)
learner_lm <- mlr3::lrn("regr.lm")

# Train and predict
learner_lm$train(task_abalone)
pred_lm <- learner_lm$predict(task_abalone)

# Inspect predictions
head(data.frame(
  id = 1:length(pred_lm$truth),
  truth = pred_lm$truth,
  response = pred_lm$response))

##   id truth response
```

```
## 1  1    15 8.840042
## 2  2     7 7.395659
## 3  3     9 9.821995
## 4  4    10 8.683616
## 5  5     7 7.160333
## 6  6     8 8.334876
```

d)
```
library(mlr3viz)

# Get nice visualization with a one-liner
mlr3viz::autoplot(pred_lm)
```



We see a scatterplot of true vs predicted values, where the small bars along the axes (a so-called rugplot) indicate the number of observations that fall into this area. As we might have suspected from the first plot, the underlying relationship is not exactly linear (ideally, all points and the resulting line should lie on the diagonal). With a linear model we tend to underestimate the response.

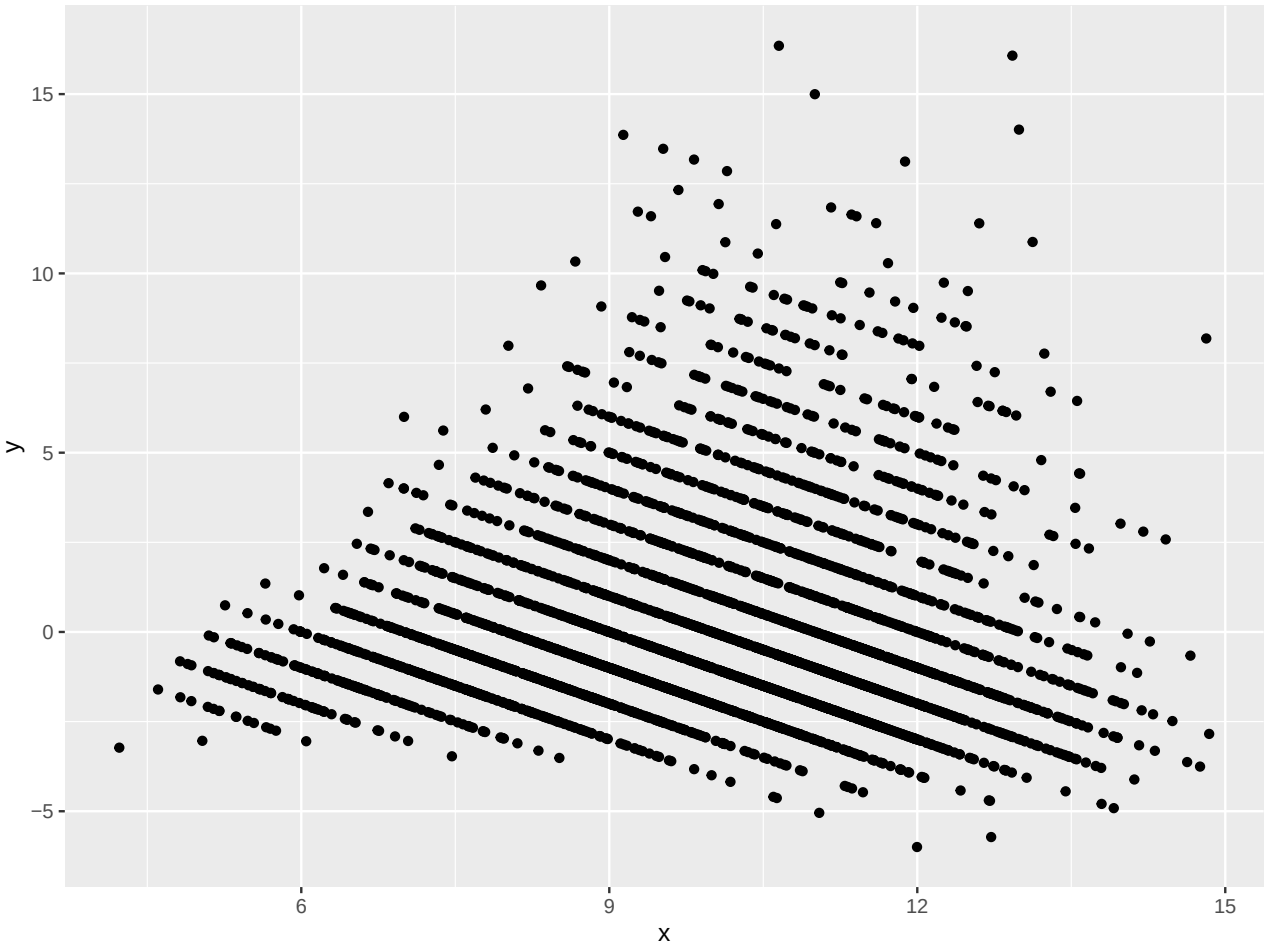
e)
```
# Define MAE metric
mae <- mlr3::msr("regr.mae")

# Assess performance (MSE by default)
pred_lm$score()

## regr.mse
## 7.125521
```

```
pred_lm$score(mae)

## regr.mae
##  1.95066
```

*) While we focus on "learning to predict" here, we can of course also do the usual model interpretation, e.g., examining the coefficients.

All effects highly significant:

```
summary(learner_lm$model)

##
## Call:
## stats::lm(formula = task$formula(), data = task$data())
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -5.9976 -1.6747 -0.7428  0.9122 16.3478
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)     3.4313     0.3156   10.87  < 2e-16 ***
## longest_shell  10.5824     0.9071   11.67  < 2e-16 ***
## whole_weight    1.1550     0.2221    5.20 2.09e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.67 on 4174 degrees of freedom
## Multiple R-squared:  0.3144,Adjusted R-squared:  0.314
## F-statistic: 956.9 on 2 and 4174 DF,  p-value: < 2.2e-16

# Not-so-homoskedastic residuals
ggplot2::ggplot(
  data.frame(
    x = learner_lm$model$fitted.values,
    y = learner_lm$model$residuals),
  aes(x, y)) +
  ggplot2::geom_point()
```



See also R file