K-Fold Cross Validation

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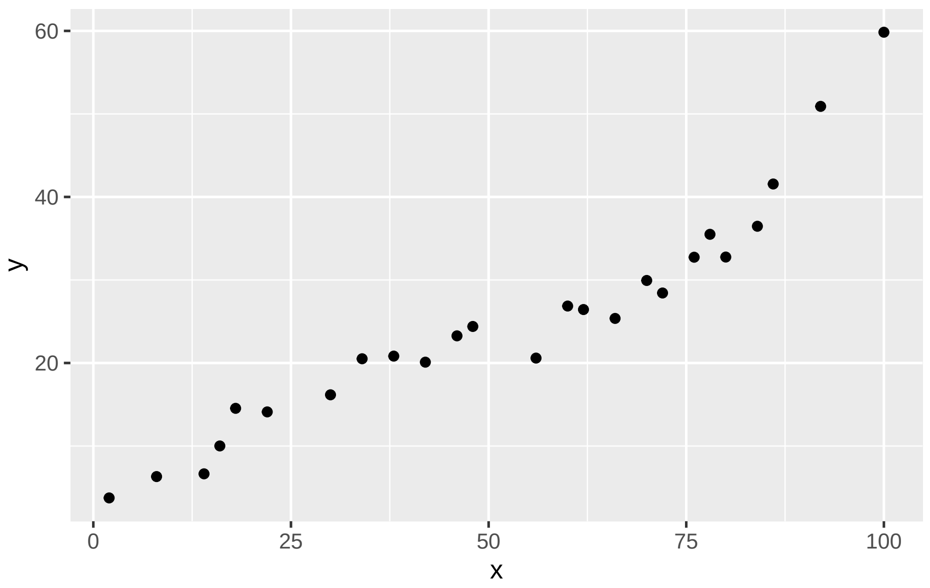
1 Loading the data

We load the data from a web address and make a quick plot:

```
data <- read_csv("https://paolobosetti.quarto.pub/data/kfold.csv",
                 show_col_types = FALSE)
data %>% ggplot(aes(x=x, y=y)) + geom_point()
```



2 Linear model regression

The regression of a linear model is performed with the `lm()` function. It takes two arguments:

- a **formula**, i.e. a description of the regression model
- a **data table**, containing the data set to use for regression. The columns of the data set must have the same names used for the predictors

The formula is expressed in the **formula notation**, which is a map from an analytical regression model, as $y_i = a + bx_i + cx_i^2 + \varepsilon_i$ to a formula object as `y~x + I(x^2)`

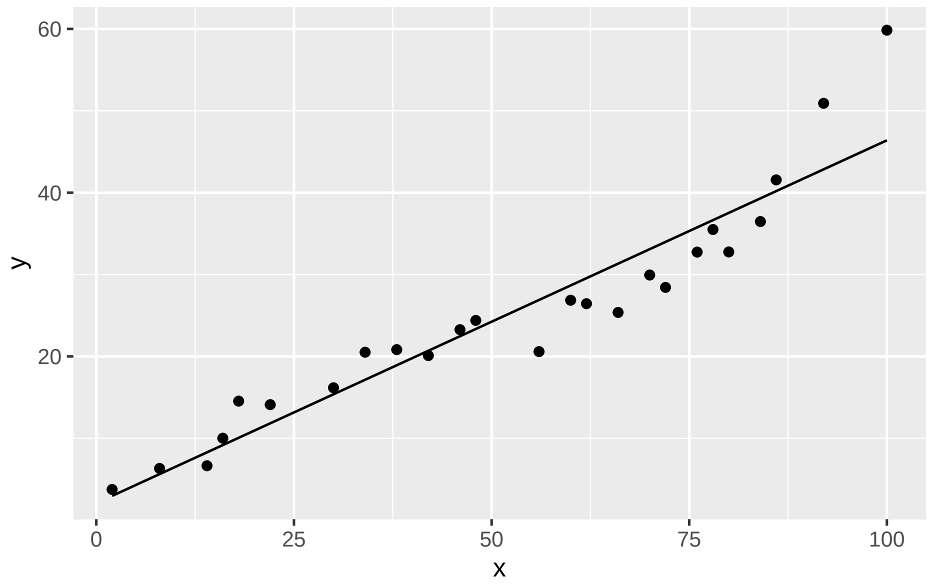
To build a formula from a model you typically:

- drop the grand average a and the residuals ε_i
- when you need the power of a term (or any mathematical function applied to a term like a logarithm), you have to protect it with the identity function `I()`
- if you have more than one predictor, you can combine them as `y~x1 + x2`, which corresponds to $y_i = a + bx_{1,i} + cx_{2,1} + \varepsilon_i$ or as `y~x1 + x2 + x1:x2`, which corresponds to $y_i = a + bx_{1,i} + cx_{2,1} + dx_{1,i}x_{2,i} + \varepsilon_i$
- the notation `y~x1 + x2 + x1:x2` can be abbreviated as `y~x1*x2`
- to remove from the model the grand average (called *intercept*), subtract 1: $y_i = bx_i + cx_i^2 + \varepsilon_i$ becomes `y~x + I(x^2) - 1`

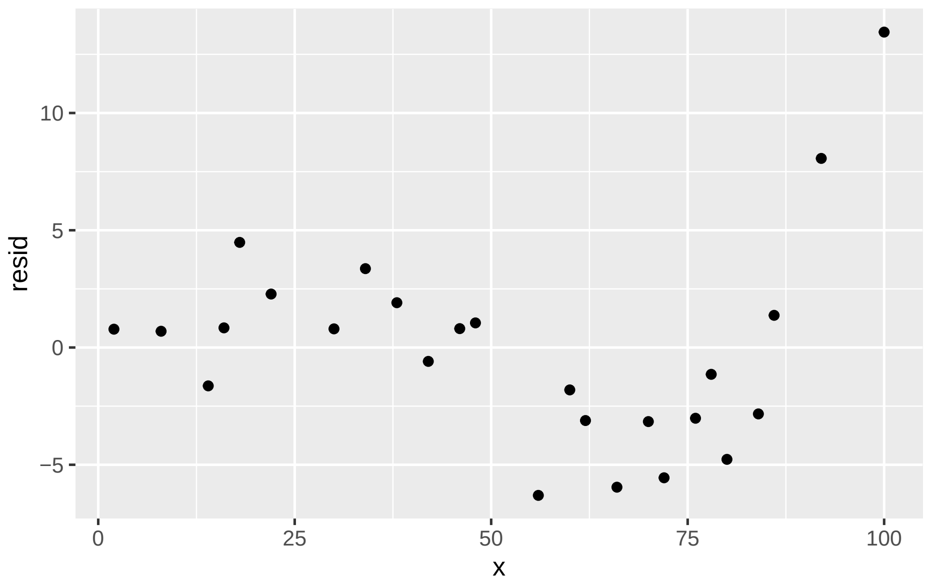
So let’s build a linear model of degree 2:

```r
data.lm <-lm(y~x, data=data)

data %>%
  add_predictions(data.lm) %>%
  ggplot(aes(x=x)) +
  geom_point(aes(y=y)) +
  geom_line(aes(y=pred))
```



```r
data %>%
  add_residuals(data.lm) %>%
  ggplot(aes(x=x, y=resid)) +
  geom_point()
```



We note that the residuals show a rather strong pattern, meaning that the linear relationship is underfitting the data, and thus we need to increase the degree of the fitting polynomial. But how much so?

3 Multiple regressions

The degree of the fitting polynomial is a **hyper-parameter**. In fact, regression **parameters** are the coefficients of the polynomial, to be calculated typically by minimizing the root mean square of the residuals. But the degree of the polynomial is a parameter that defines the **number** of regression parameters, and that is why it is named a **hyper-parameter**. Identifying the best hyper-parameter(s) is the aim of validation and cross-validation strategies.

In our case we want to compare polynomial fits up to degree 12, using a `map`:

```r
fits <- 1:12 %>%
  map(\(deg) lm(y~poly(x, deg, raw=T), data = data))
```

Quality of a regression can be verified with different metrics:

- $R^2 = 1 - \frac{\sum(x_i - \hat{x}_i)^2}{\sum(x_i - \bar{x}_i)^2}$
- $\mathrm{MSE} = \frac{\sum(x_i - \hat{x}_i)^2}{N}$
- $\mathrm{RMSE} = \sqrt{\frac{\sum(x_i - \hat{x}_i)^2}{N}}$
- $\mathrm{MAE} = \frac{\sum|x_i - \hat{x}_i|}{N}$
- $\mathrm{MAPE} = \frac{1}{N}\sum\left|\frac{x_i - \hat{x}_i}{x_i}\right|$

Typically, the root means square of error (RMSE) and the mean absolute error

(MAE) are the most commonly used metrics.

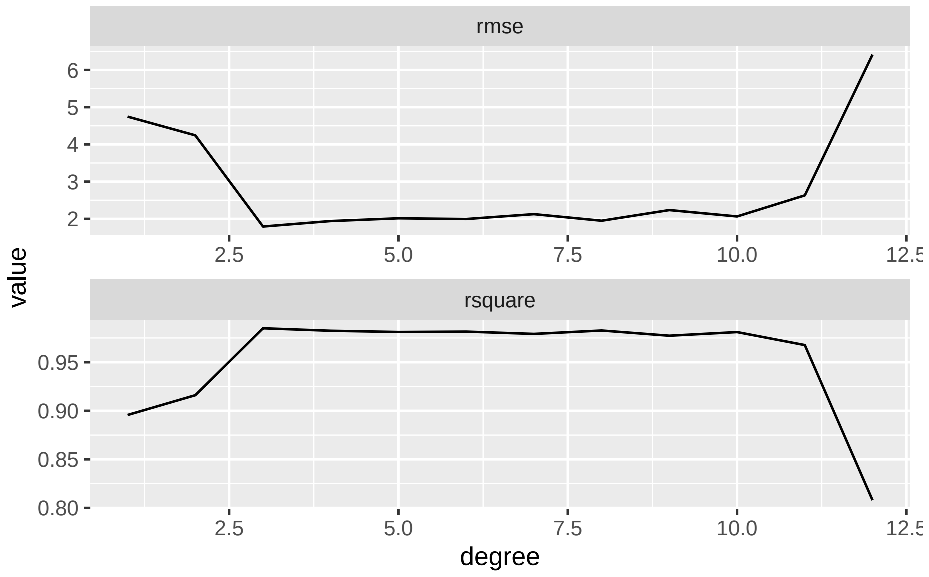
Let's see how the RMSE and the R^2 metrics change when the polynomial degree increases. To do that we build a table with three columns:

1. the degree of the polynomial
2. the R^2 value
3. the RMSE value

We extract these data from the list of linear models above created, `fits`. For each fitted linear model (an entry in `fits`), the R^2 and RMSE can be extracted with the functions `rsquare()` and `rmse()`, respectively.

We use `map_dbl()` to map these functions over the list of polynomial degrees. The resulting table is then used to make a plot:

```r
tibble(
  degree=1:12, # deg starts from 2!
  rsquare=fits %>% map_dbl(~rsquare(., df)),
  rmse=fits %>% map_dbl(~rmse(., df))
) %>%
  pivot_longer(-degree, names_to = "Index") %>%
  ggplot(aes(x=degree, y=value)) +
  geom_line() +
  facet_wrap(~Index, nrow=2, scales="free")
```



The R^2 increases pretty quickly and saturates after degree 3. The RMSE decreases sharply and monotonically. It's hard to figure out the point where over-fitting starts.

4 K-fold cross-validation

To solve the problem we use K-fold cross validation. It is a regression strategy where we split the dataset into k subsets, or *folds*, with roughly the same amount of observations. Then:

- we train the model over all the folds together **except the first fold**, and then we validate the model on the first model, i.e. we calculate one or more metrics on the validation data
- we repeat the previous step setting aside each fold, one at a time, and using it for validation, while the remaining folds are used for training
- each fold is used exactly once for validation, exactly $k-1$ times for training
- we calculate the overall metrics, by calculating the average of the k metrics evaluated for each validation step, or — equivalently — by appliying the above reported equations to the whole set of validation values

In R, we use the `caret` library to simplify this process. The `caret::train()` function performs the folding for a given model: it takes as arguments the model formula, the regression function (in our case `lm()`), the dataset, and a list of parameters that can be created with the supporting `trainControl()` function.

The `trainControl()` function is used to define the details on the cross validation strategy to use. In our case we use the **repeated** K-fold cross validation, named `"repeatedcv"`, which repeates a K-fold a given number of times.

In fact, the folds are defined by randomly sampling the initial dataset, so that the resulting RMSE (or any other metric) is also a random variable. Repeating the K-fold 100 times makes the whole process more robust:

```r
ctrl <- trainControl(method = "repeatedcv", number=5, repeats=100)
model <- train(y~poly(x,8), data=data, method="lm", trControl=ctrl)

model
```

```
Linear Regression

25 samples
 1 predictor

No pre-processing
Resampling: Cross-Validated (5 fold, repeated 100 times)
Summary of sample sizes: 20, 20, 21, 20, 19, 20, ...
Resampling results:

  RMSE     Rsquared   MAE
  10.3213  0.9241026  6.25129

Tuning parameter 'intercept' was held constant at a value of TRUE
```

The `model` object contains a field named `model$results` that is a table with all the available performance metrics:

intercept	RMSE	Rsquared	MAE	RMSESD	RsquaredSD	MAESD
TRUE	10.3213	0.9241026	6.25129	23.37541	0.1183862	12.14192

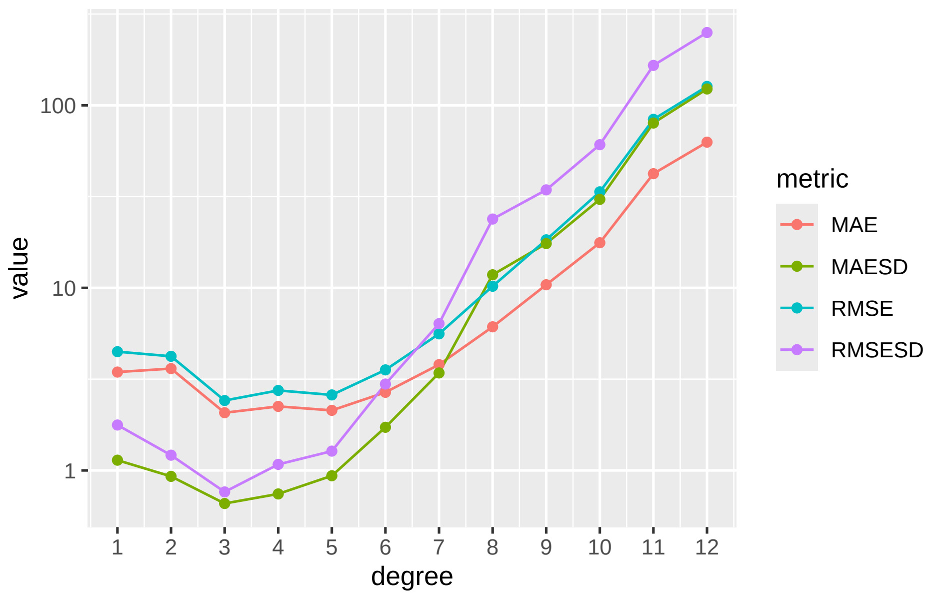
Now we want to repeat the K-fold validation over the list of formulas corresponding to the set of polynomials with degrees from 1 to 12. We use again the `map()` function:

```r
fit_quality <- tibble(
  degree=1:12,
  results=map(degree, \(n) {
    fm <- paste0("y~poly(x,", n, ", raw=TRUE)") %>% as.formula()
    train(fm, data=data, method="lm", trControl=ctrl)$results
    })
) %>%
  unnest(cols=results)
```

Note the `unnest()` function at the end: the model field `$results` is actualy a table, so without that function in `fit_quality` we would get a column `results` that contains a list of tables. The `unnest()` function flattens this list of tables in place.

Now we can finally make a plot of the metrics as a function of the polynomial degree:

```r
fit_quality %>%
  select(-intercept, -starts_with("Rsquared")) %>%
  pivot_longer(-degree, names_to = "metric") %>%
  ggplot(aes(x=degree, y=value, group=metric, color=metric)) +
  geom_line() +
  geom_point() +
  scale_y_log10() +
  scale_x_continuous(breaks=1:12)
```



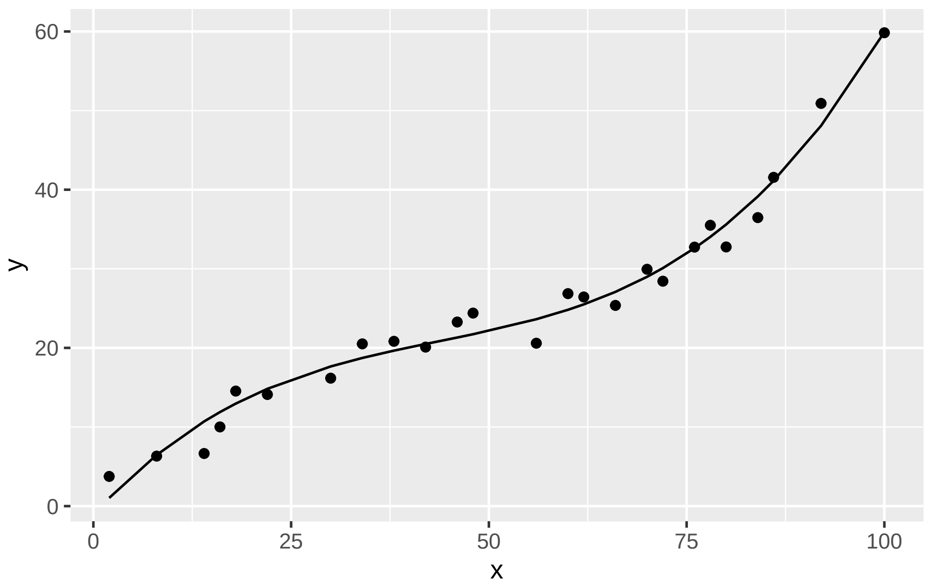
We observe that the minima of any metric happens at degree 3. This means that below that value we have underfitting, above we have overfitting (i.e. the model is loosing generality).

5 Regression

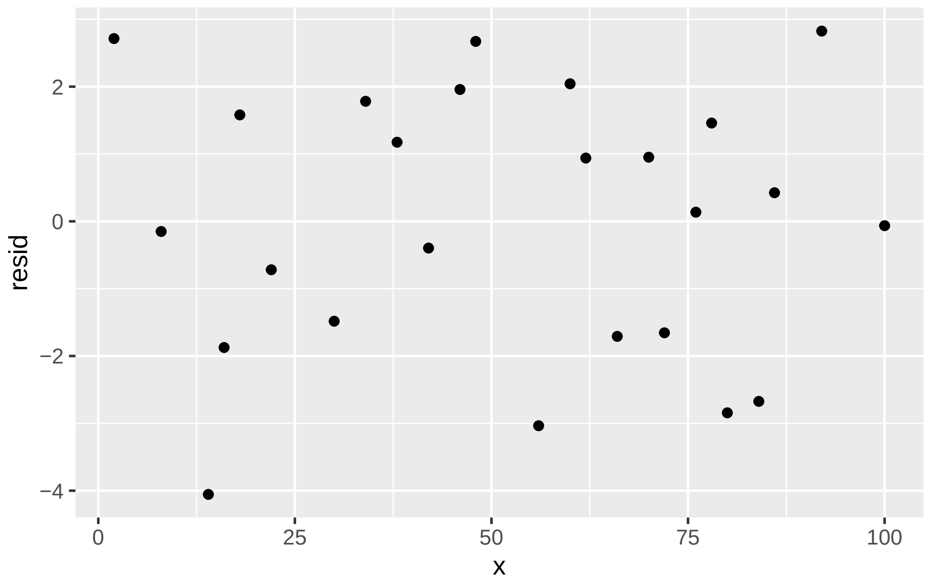
So we can finally accept the model $y_i = a + bx_i + cx_i^2 + dx_i^3 + \varepsilon_i$ (a degree 3 polynomial in x_i):

```r
data.lm <- lm(y~poly(x, 3), data=data)

data %>%
  add_predictions(data.lm) %>%
  ggplot(aes(x=x, y=y)) +
  geom_point() +
  geom_line(aes(y=pred))
```

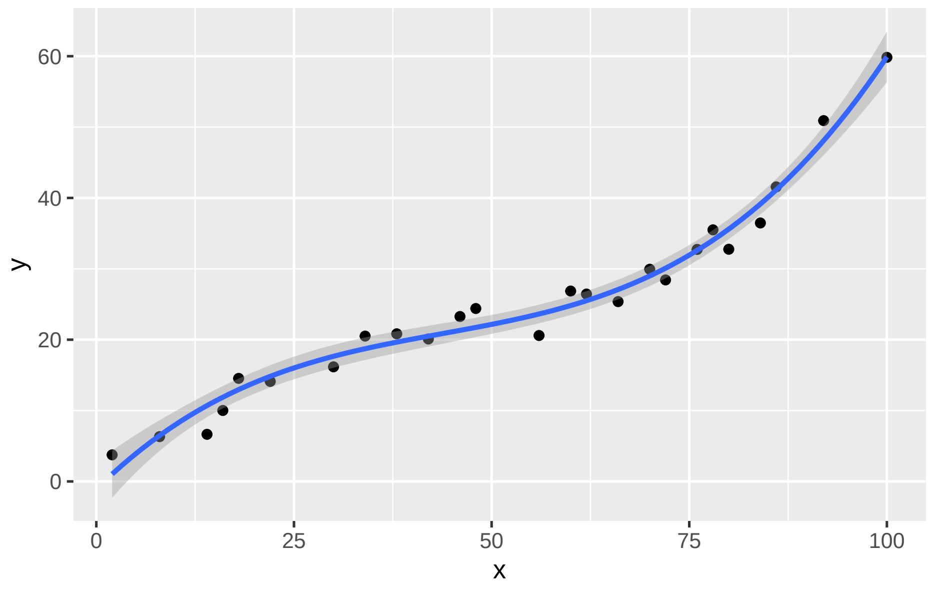


```
data %>%
  add_residuals(data.lm) %>%
  ggplot(aes(x=x, y=resid)) +
  geom_point()
```



We confirm that the residuals are free from patterns. We can also plot a confidence interval of the same regression by using the `geom_smooth()` layer in a `ggplot`:

```r
data %>%
  ggplot(aes(x=x, y=y)) +
  geom_point() +
  geom_smooth(method="lm", formula=y~poly(x, 3))
```


60
40
20
0
y
0
25
50
75
100
x