Module 2: STATISTICAL LEARNING

TMA4268 Statistical Learning V2018

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week 3 2018 (Version 27.04.2018)

Contents

Last changes: (18.01: corrected error on sd=2 and not sd=1 in simulations for Bias-variance irreducible error. 20.01: corrected answer to quiz on mvN and added some more answers. 21.01: Moved needed packages to the end of the page. 24.04: typos and html toc added.)

Aim of the module

- Statistical learning and examples thereof
- Introduce relevant notation and terminology.
- Estimating f (regression, classification): prediction accuracy vs. model interpretability
- Bias-variance trade-off
- Classification:
  - The Bayes classifier
  - K nearest neighbour (KNN) classifier
- The basics of random vectors, covariance matrix and the multivariate normal distribution.

Learning material for this module:

- James et al (2013): An Introduction to Statistical Learning. Chapter 2.

- Additional material (in this module page) on random variables, covariance matrix and the multivariate normal distribution (known for students who have taken TMA4267 Linear statistical models).

Added after the lecture:

- Classnotes 15.01.2018.

Move to:

- Part A: Statistical learning - core concepts
- Part B: Random vectors, covariance matrix and the multivariate normal distribution
- Recommended exercises
- Further reading
- Packages to install before knitting this R Markdown file

Part A: Core concepts in statistical learning

What is Statistical Learning?

Statistical learning is the process of learning from data.

By applying *statistical methods* (or algorithms) on a *data set* (called the *training set*), the aim is to *draw conclusions* about the relations between the variables or to *find a predictive function* for new observations.

Statistical learning plays a key role in many areas of science, finance and industry.

Variable types

Variables can be characterized as either *quantitative* or *qualitative*.

Quantitative variables are variables from a continuous set, they have a numerical value.

Examples: a person's weight, a company's income, the age of a building, the temperature outside, the amount of rainfall etc.

Qualitative variables are variables from a discrete set, from a set of K different classes/labels/categories.

Examples of qualitative variables are: type of fruit {apples, oranges, bananas, ...}, the age groups in a marathon: {(below 18), (18-22), (23 - 34), (35 - 39), (40 - 44), ... }. Qualitative variables which have only two classes are called *binary* variables and are usually coded by 0 (no) and 1 (yes).

Examples of learning problems

Economy:

To predict the price of a stock 3 months from now, based on company performance measures and economic data. Here the response variable is quantitative (price).

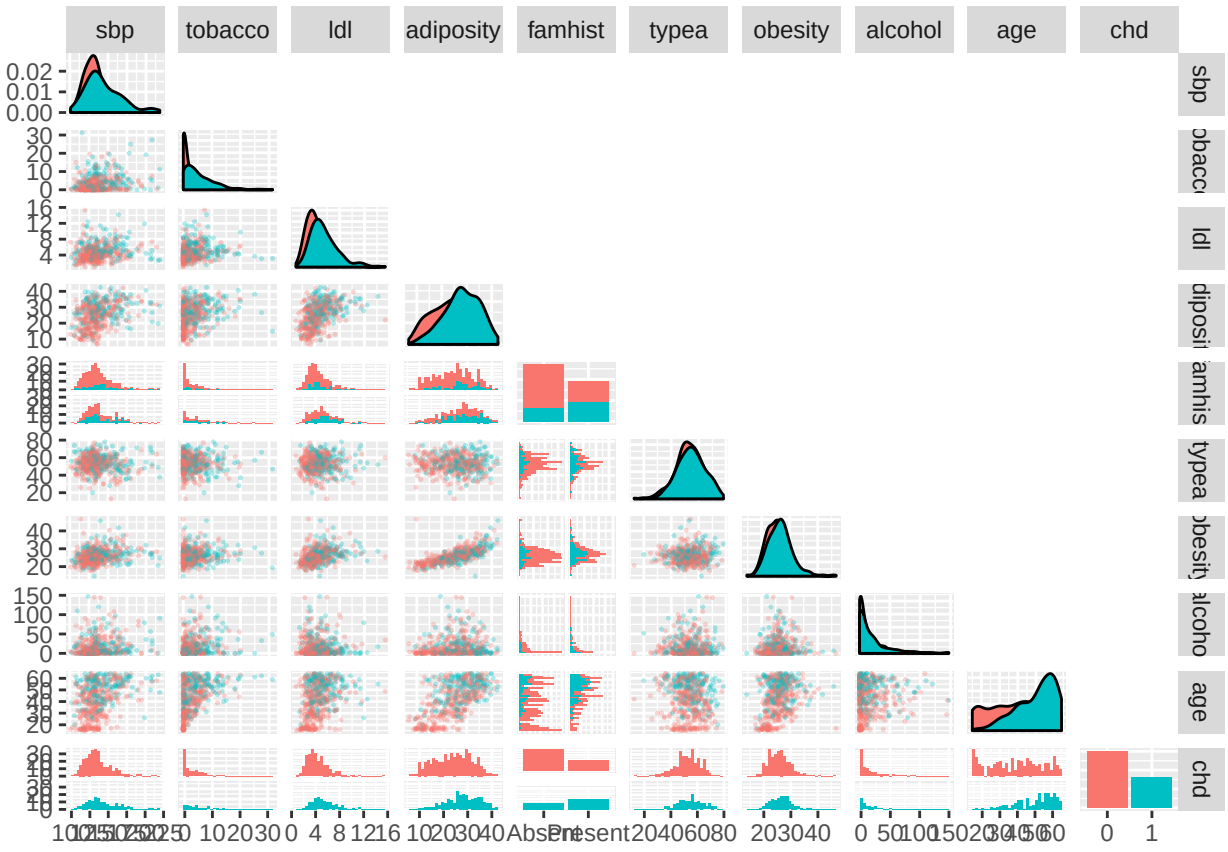
Medicine 1:

To identify the risk factors for developing diabetes based on diet, physical activity, family history and body measurements. Here the aim is to make inference of the data, i.e. to find underlying relations between the variables.

Medicine 2:

To predict whether someone will suffer a heart attack on the basis of demographic, diet and clinical measurements. Here the outcome is binary (yes,no) with both qualitative and quantitative input variables.

South African heart disease data: 462 observations and 10 variables.



Handwritten digit recognition:

To identify the numbers in a handwritten ZIP code, from a digitized image. This is a classification problem, where the response variable is categorical with classes $\{0, 1, 2, \ldots, 9\}$ and the task is to correctly predict the class membership.

Examples of handwritten digits from U.S. postal envelopes. Image taken from https://web.stanford.edu/~hastie/ElemStatLearnII/

Email classification (spam detection):

The goal is to build a spam filter. This filter can based on the frequencies of words and characters in emails. The table below show the average percentage of words or characters in an email message, based on 4601 emails of which 1813 were classified as a spam.

	you	free	george	!	$	edu
not spam	1.27	0.07	1.27	0.11	0.01	0.29
spam	2.26	0.52	0.00	0.51	0.17	0.01

What makes a Nobel Prize winner?

Perseverance, luck, skilled mentors or simply chocolate consumption? An article published in the New England Journal of Medicine have concluded with the following:

> Chocolate consumption enhances cognitive function, which is a sine qua non for winning the Nobel Prize, and it closely correlates with the number of Nobel laureates in each country. It remains to be determined whether the consumption of chocolate is the underlying mechanism for the observed association with improved cognitive function.

The figure shows the correlations between a countries' annual per capita chocolate consumption and the number of Nobel Laureates per 10 million population.

You can read the article here and a informal review of the article here.

Hopefully we will not run out of chocolate already in 2020

Q: Were there common underlying aims and elements of these examples of statistical learning?

- To predict the price of a stock 3 months from now, based on company performance measures and economic data.
- To identify the risk factors for developing diabetes based on diet, physical activity, family history and body measurements.
- The goal is to build a spam filter.
- To predict whether someone will suffer a heart attack on the basis of demographic, diet and clinical measurements.
- To identify the numbers in a handwritten ZIP code, from a digitized image.
- What makes a Nobel Prize winner? Perseverance, luck, skilled mentors or simply chocolate consumption?

A: yes, the aim was either understanding or prediction, some output variables were continuous others were discrete.

What is the aim in Statistical learning?

Assume:

- we observe one *quantitative* response Y and
- p different predictors $x_1, x_2, ..., x_p$.

We assume that there is a function f that relates the response and the predictor variables:

$$Y = f(x) + \varepsilon,$$

where ε is a random error term with mean 0 and independent of x.

There are two main reasons for estimating f: *prediction and inference*

Prediction

Based on observed data the aim is to build a model that as accurately as possible can predict a response given new observations of the covariates:

$$\hat{Y} = \hat{f}(x).$$

Here $\hat{f}$ represents the estimated f and $\hat{Y}$ represents the prediction for Y. In this setting our estimate of the function f is treated as a **black box and is not of interest**. Our focus is on the prediction for Y, hence prediction accuracy is important.

There are two quantities which influence the accuracy of $\hat{Y}$ as a prediction of Y: the reducible and the irreducible error.

- The *reducible error* has to do with our estimate $\hat{f}$ of f. This error can be reduced by using the most *appropriate* statistical learning technique.
- The *irreducible error* comes from the error term ε and cannot be reduced by improving f. This is related to the unobserved quantities influencing the response and possibly the randomness of the situation.

Inference

Based on observed data the aim is to *understand* how the response variable is affected by the various predictors (covariates).

In this setting we will not use our estimated function $\hat{f}$ to make predictions but to *understand* how Y changes as a function of $x_1, x_2, ..., x_p$.

The *exact form* of $\hat{f}$ is of *main interest*.

- Which predictors are associated with the response?
- What is the relationship between the response and each predictor?
- Can the relationship be linear, or is a more complex model needed?

The difference between Statistical Learning and Machine Learning

There is much overlap between statistical learning and machine learning: the common objective is learning from data. Specifically, to find a target function f that best maps input variables x to an output variable Y: $Y = f(x)$.

This function f will allow us to make a prediction for a future Y, given new observations of the input variables x's.

- Machine learning arose as a subfield of artificial intelligence and has generally a greater emphasis on *large scale applications and prediction accuracy*, the shape and the form of the function f is in itself (generelly) not interesting.
- Statistical learning arose as a subfield of statistics with the main focus on model *interpretability*.

Naming convention

Statistical Learning	Machine Learning
model	network, graph, mapping

Statistical Learning	Machine Learning
fit, estimate	learn
covariates, inputs, independent variables, predictors	features, predictors
response, output, dependent variable	output, target
data set	training data

Remark: not an exhaustive list, and common usage of many terms.

Regression and classification

Regression predicts a value from a continuous set.

Classification predicts the class membership.

Q:

Give an example of one regression and one classification problem (practical problem with data set available) that you would like to study in this course.

A: See classnotes for suggestions in class.

Supervised and unsupervised learning

Supervised learning

Our data set (training set) consists of n measurement of the response variable Y and of p covariates x:

$$(y_1, x_{11}, x_{12}, \ldots, x_{1p}), (y_2, x_{21}, \ldots, x_{2p}), \ldots, (y_n, x_{n1}, x_{n2}, \ldots, x_{np}).$$

Aim:

- make accurate predictions for new observations,
- understand which inputs affect the outputs, and how, and
- to assess the quality of the predictions and inference. It is called supervised learning because the response variable *supervises our analysis*.

Examples (we will study):

- Linear regression (M3), Logistic regression (M4), Generalized additive models (M7)
- Classification trees, bagging, boosting (M8), K-nearest neighbor classifier (M2,M4)
- Support vector machines (M9)

Unsupervised learning

Our data set now consists of input measurements, x_i's, but without labelled responses y_i's.

The aim is to find (hidden) patterns or groupings in the data - in order to *gain insight and understanding*. There is no *correct* answer.

Examples:

- Clustering (M10), Principal component analysis (M10)
- Expectation-maximization algorithm (TMA4300)

Semi-Supervised Learning

Our data set consists of a input data, and some of the data has labelled responses. This situation can for example occur if the measurement of input data is cheap, while the output data is expensive to collect. Classical solutions (likelihood-based) to this problem exists in statistics (missing at random observations).

Q:

Explain to your neighbour the difference between supervised and unsupervised learning by the use of examples.

Models and methods

Parametric Methods

Parametric methods build on an assumption about the form or shape of the function f.

The multiple linear model (Module 3) is an example of a parametric method. We here assume that the response variable is a linear combination of the covariates

$$f(x) = \beta_0 + \beta_1 x_1 + ... + \beta_p x_p.$$

By making this assumption, the task simplifies to finding estimates of the $p + 1$ coefficients $\beta_0, \beta_1, .., \beta_p$. To do this we use the training data to fit the model, such that

$$Y \approx \beta_0 + \beta_1 x_1 + ... + \beta_p x_p.$$

Fitting a parametric models is thus done in two steps:

1. Select a form for the function f.

2. Estimate the unknown parameters in f using the training set.

Non-parametric methods

Non-parametric methods seek an estimate of f that gets close to the data points, but without making explicit assumptions about the form of the function f.

The K-nearest neighbour algorithm is an example of a non-parametric model. This algorithm predicts a class membership for a new observation by making a majority vote based on its K nearest neighbours. We will discuss the K-nearest neighbour algorithm later in this module.

Q:

What are the advantages and disadvantages of parametric and non-parametric methods?

Hints: interpretability, amount of data needed, complexity, assumptions made, prediction accuracy, computational complexity, over/under-fit.

Parametric methods

Advantages	Disadvantages
Simple to use and easy to understand	The function f is constrained to the specified form.
Requires little training data	The assumed function form of f will in general not match the true function, potentially giving a poor estimate.
Computationally cheap	Limited complexity

Non-parametric methods

Advantages	Disadvantages
Flexible: a large number of functional forms can be fitted	Can overfit the data
No strong assumptions about the underlying function are made	Computationally more expensive as more parameters need to be estimated
Can often give good predictions	Much data is required to estimate (the complex) f.

Prediction accuracy vs. interpretability

Inflexible, or rigid, methods are methods which have high restrictions on the shape of f.

Examples:

- Linear regression (M3)
- Linear discriminant analysis (M4)
- Subset selection and lasso (M6)

Flexible methods allow for the shape of f from a wider range.

Examples:

- KNN classification (M2,M4)
- Smoothing splines (M7)
- Bagging and boosting (M8), support vector machines (M9)

The choice of a flexible or inflexible method depends on the goal in mind.

If the aim is inference an inflexible model, which is easy to understand, will be preferred. On the other side, if we want to make as accurate predictions as possible, we are not concerned about the shape of f. A flexible method can be chosen, at the cost of model interpretability, and we treat f like a black box.

Overfitting occurs when the estimated function f is too closely fit to the observed data points.

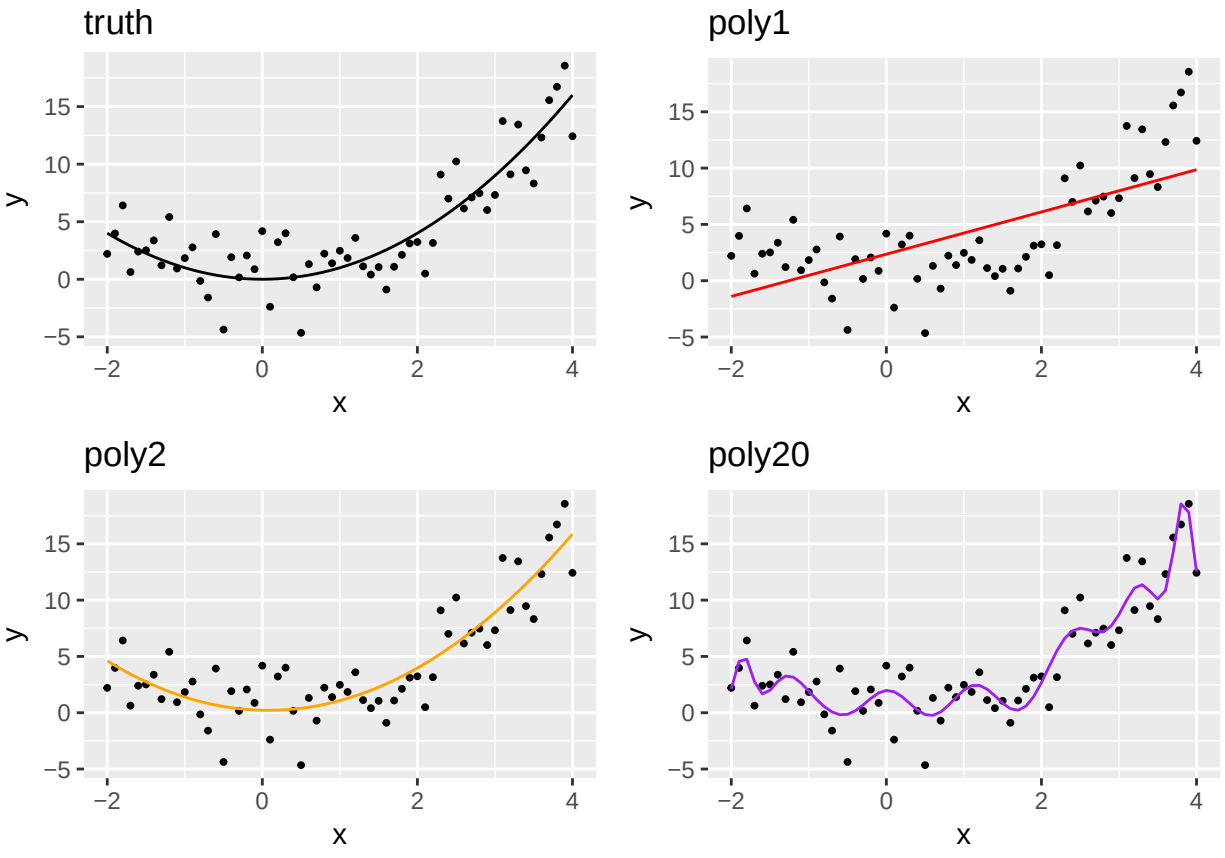
Underfitting occurs when the estimated function f is too rigid to capture the underlying structure of the data.

We illustrate this by a toy example with four figures. The black line in the first figure shows the function from which we have simulated theoretical observations: $y = x^2$. The black dots show the "observed" values. These have been simulated by adding normal noise (mean 0 and standard deviation 2) to the original equation. x-values are chosen in the real line from -2 to 4, equally spaced at 0.1, giving $n = 61$.

Now, assume that the black dots are observations to which you want to fit a function *without* knowing the true relationship.

- The red line shows a simple linear model of the form $\beta_0 + \beta_1 x$ fitted to the observations. This line clearly underfits the data. We see that this function is unable to capture that convex nature of the data.
- The orange line shows a quadratic polynomial fit to the data, of the form $\beta_0 + \beta_1 x + \beta_2 x^2$. We see that this function fits well and looks almost identically as the true function.
- The purple line shows a polynomial of degree 20 fit to the data, of the form $\beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_{20} x^{20}$. We here observe overfitting. The function captures the noise instead of the underlying structure of the data.

We will discuss polynomial regression in Module 7.

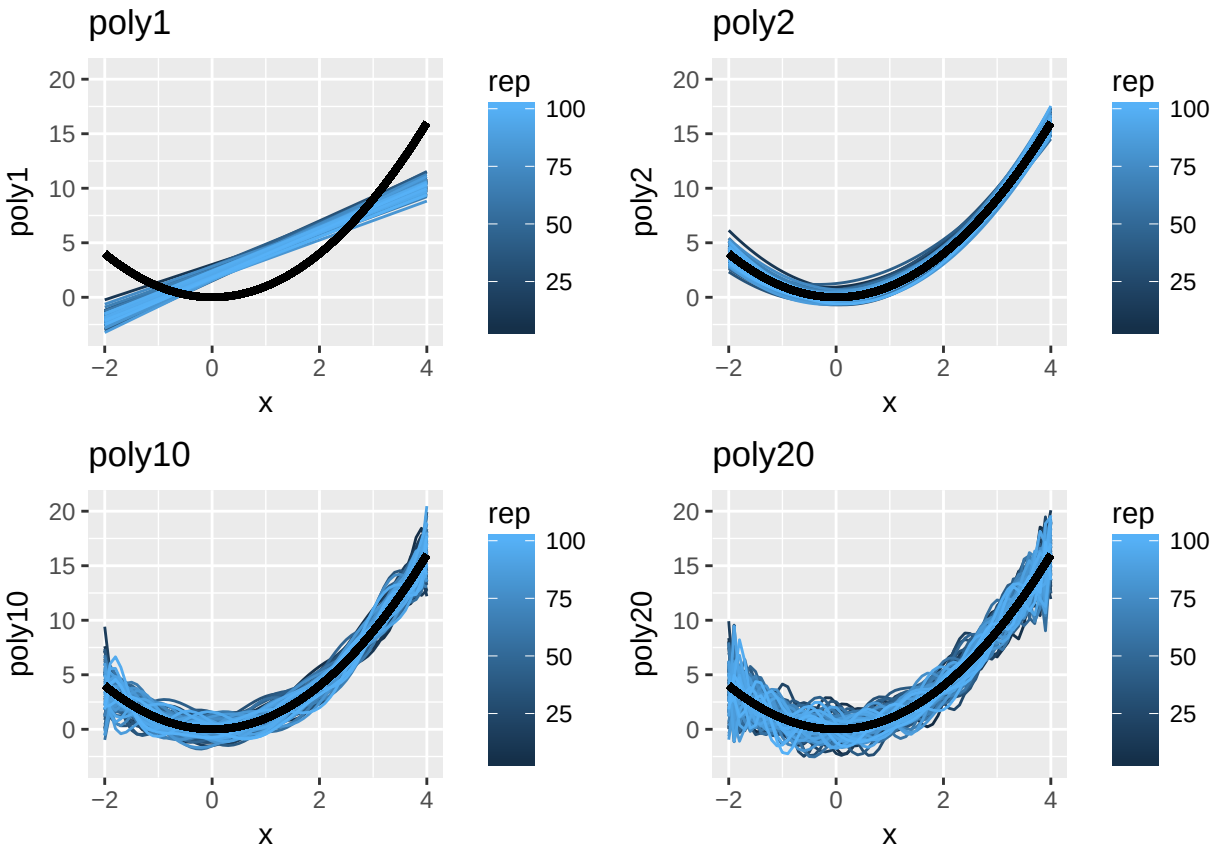


Q: The coloured curves are our estimates for the functional relationship between x and Y.

- Which of the coloured curves does the best job? Rank the curves.
- Now only consider the red (order 1) and purple (order 20) models: We collect new data (of the same size with normally distributed errors) - and estimate new curves. Which of the coloured curves would on average give the best performance?
- What did you here choose to define as "best performance"?

A: See classnotes for suggestions in class.

Why comparing regressions with different degrees of polynomials? We will study several methods that includes a parameter controlling the flexibility of the model fit - so generalizations of our example with degrees for the polynomials. The K in K-nearest neighour is such a parameter. We need to know how to choose this flexibility parameter.



Kept x fixed and drew new errors 100 times. The 100 fitted curves shown. Added poly10 - to see trend from poly2 to poly20.

Loss function

Q: How can we measure the *loss* between a predicted response $\hat{y}_i$ and the observed response y_i?

A: Possible loss functions are:

- absolute loss (L1 norm): $\mid y_i - \hat{y}_i \mid$
- quadratic loss (L2 norm): $(y_i - \hat{y}_i)^2$

- 0/1 loss (categorical y): loss=0 if $\hat{y}_i = y_i$ and 1 else

Issues: robustness, stability, mathematical aspect.

We will use quadratic loss now.

Assessing model accuracy - and quality of fit

Q: For regression (or classification) in general: will there be *one* method that dominates all others?

A: No method dominates all others over all possible data sets.

- That is why we need to learn about many different methods.
- For a given data set we need to know how to decide which method produces the *best* results.
- How close is the predicted response to the true response value?

Training MSE

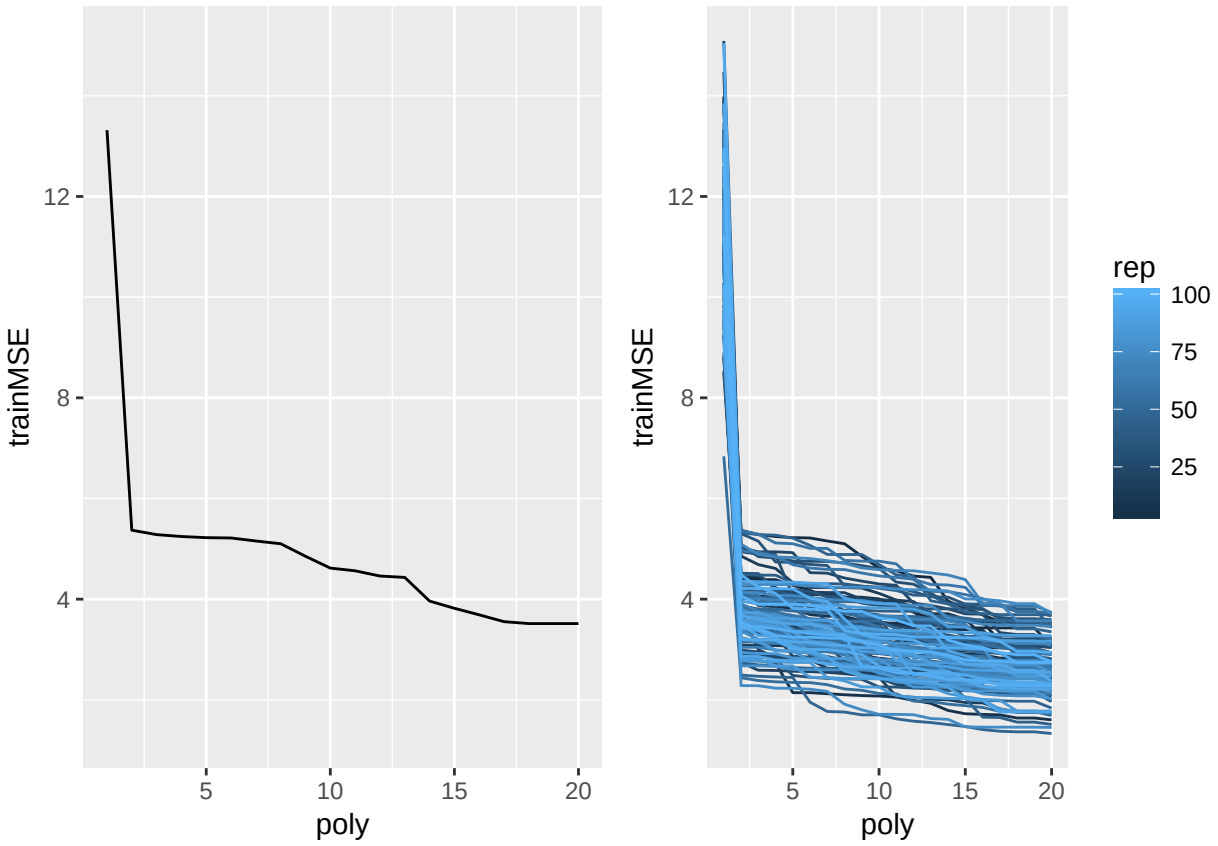
In regression, where we assume $Y = f(x) + \varepsilon$, and $\hat{f}(x_i)$ gives the predicted response at x_i, a popular measure is the *training MSE* (mean squared error): mean of squared differences between prediction and truth for the training data (the same values that were used to estimate f):

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

But, really - we are *not* interested in how the method works on the training data (and often we have designed the method to work good on the training data already), we want to know how good the method is when we use it on *previously unseen test data*.

Example:

- we don't want to predict last weeks stock price, we want to predict the stock price next week.
- we don't want to predict if a patient in the training data has diabetes, we want to predict if a new patient has diabetes.



Polynomial example: fitted order 1-20 when the truth is order 2. Left: one repetition, right: 100 repetitions.

Test MSE

Simple solution: we fit different models using the training data (maybe my minimizing the training MSE) but we choose the *best* model using a separate *test set* - be calculating the *test MSE* for a set of test observations (x_0, y_0):

$$\text{Ave}(y_0 - \hat{f}(x_0))^2$$

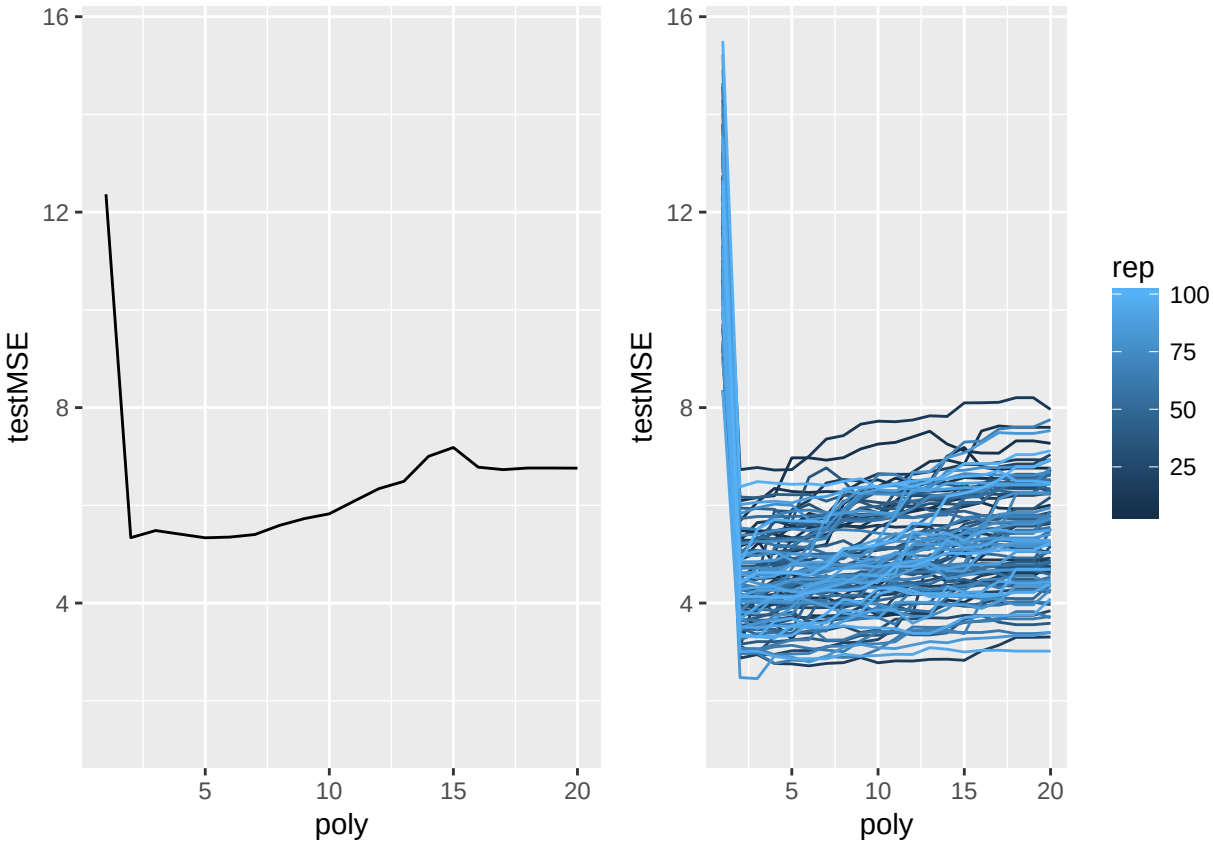
(taking the average over all available test observations).

Q: What if we do not have access to test data?

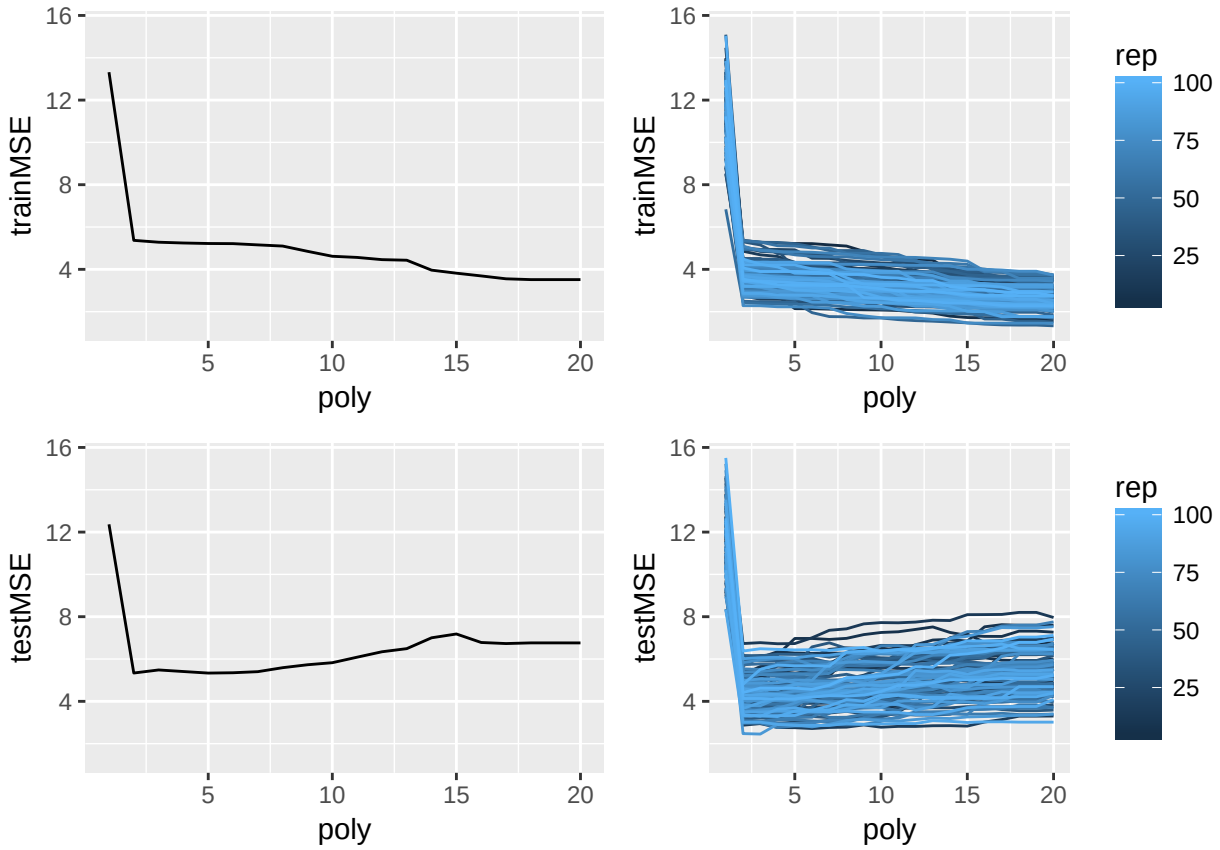
A: In Module 5 we will look into using *cross validation* to mimic the use of a test set.

Q: But, can we instead just use the training data MSE to choose a model? A low training error should also give a low test error?

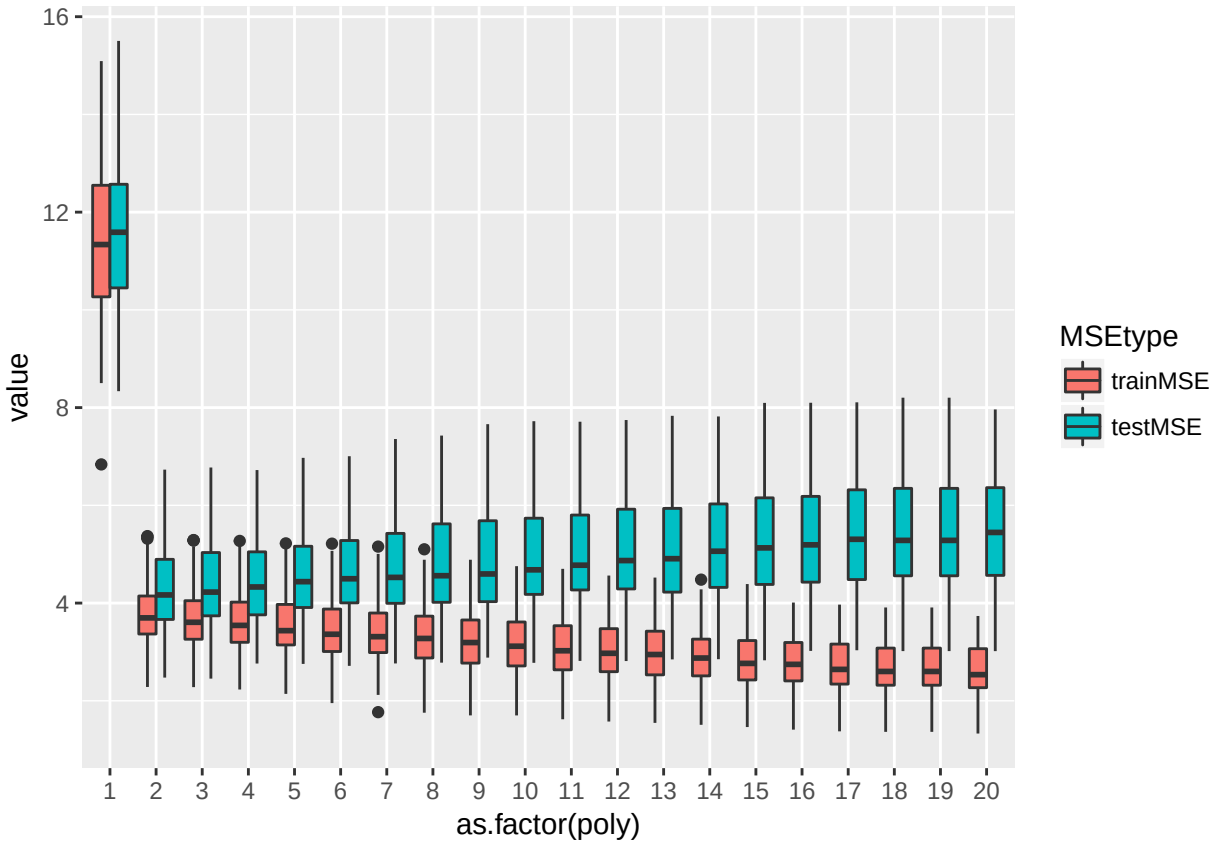
A: Sadly no, if we use a flexible model we will look at several cases where a low training error is a sign of overfitting, and will give a high test error. So, the training error is not a good estimator for the test error because it does not properly account for model complexity.



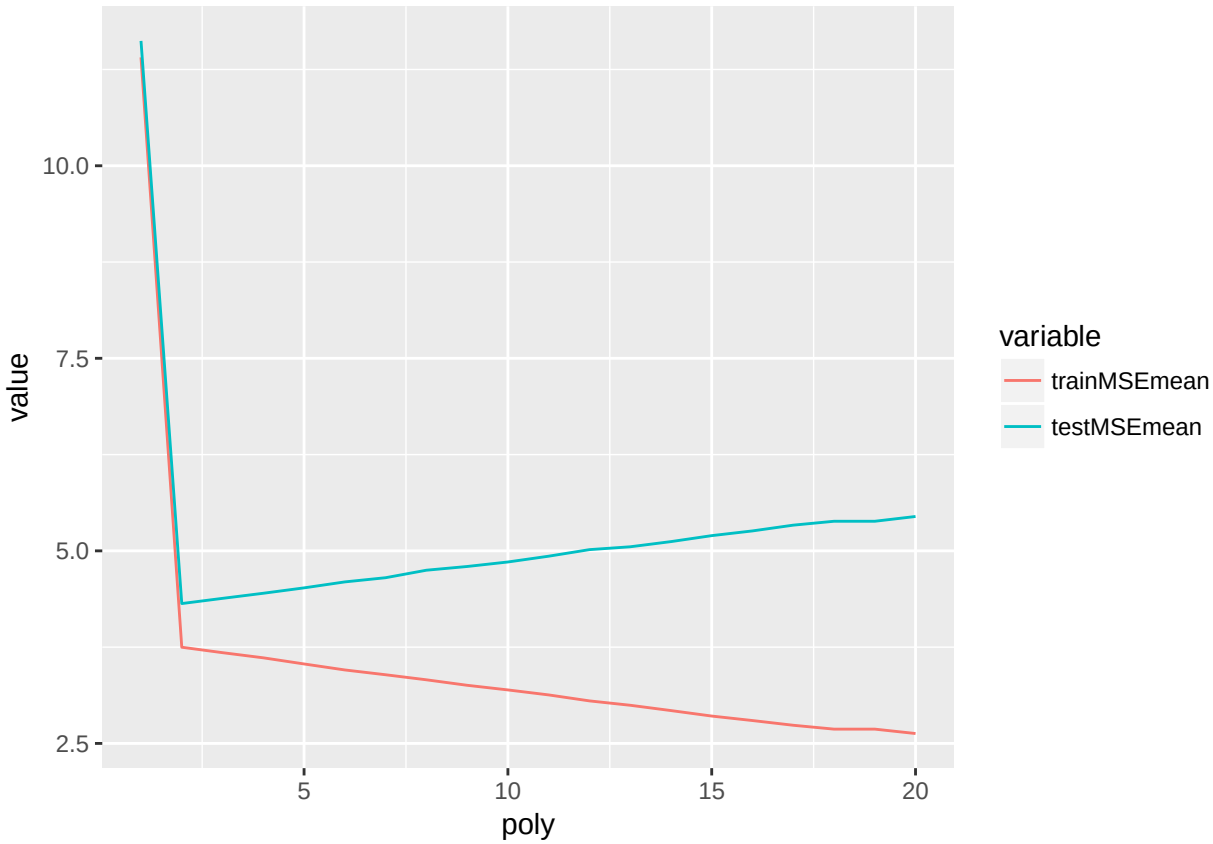
Polynomial example: fitted order 1-20 when the truth is order 2. Left: one repetition, right: 100 repetitions for the testMSE.



Polynomial example: fitted order 1-20 when the truth is order 2. Upper: trainMSE, lower: testMSE. Left: one repetition, right: 100 repetitions.



Boxplot of the 100 repetitions (polynomial experiment. Observe the U-shaped for the test error.



Mean of 100 repetitions (polynomial example). Observe U-shape. Next: We leave the trainMSE and try to understand what makes up the testMSE curve - two competing properties!

The Bias-Variance trade-off

Assume that we have fitted a *regression* curve $Y = f(x) + \varepsilon$ to our training data, which consist of independent observation pairs $\{x_i, y_i\}$ for $i = 1, .., n$. (Yes, only one x.)

We assume that ε is an unobserved random variable that adds noise to the relationship between the response variable and the covariates and is called the random error, and that the random errors have mean zero and constant variance σ^2 for all values of x.

This noise is used as a substitute for all the unobserved variables that is not in our equation, but that influences Y.

The fitted curve is denoted by $\hat{f}$.

We want to use $\hat{f}$ to make a prediction for a new observation at x_0, and are interested in the error associated with this prediction. The predicted response value is then $\hat{f}(x_0)$.

The *expected test mean squared error (MSE) at* x_0 is defined as:

$$\mathrm{E}[Y - \hat{f}(x_0)]^2$$

The *expected test mean squared error (MSE) at* x_0 is defined as:

$$\mathrm{E}[Y - \hat{f}(x_0)]^2$$

This expected test MSE can be decomposed into three terms

$$\begin{aligned}
\mathrm{E}[Y - \hat{f}(x_0)]^2 &= \mathrm{E}[Y^2 + \hat{f}(x_0)^2 - 2Y\hat{f}(x_0)] \\
&= \mathrm{E}[Y^2] + \mathrm{E}[\hat{f}(x_0)^2] - \mathrm{E}[2Y\hat{f}(x_0)] \\
&= \mathrm{Var}[Y] + \mathrm{E}[Y]^2 + \mathrm{Var}[\hat{f}(x_0)] + \mathrm{E}[\hat{f}(x_0)]^2 - 2\mathrm{E}[Y]\mathrm{E}[\hat{f}(x_0)] \\
&= \mathrm{Var}[Y] + f(x_0)^2 + \mathrm{Var}[\hat{f}(x_0)] + \mathrm{E}[\hat{f}(x_0)]^2 - 2f(x_0)\mathrm{E}[\hat{f}(x_0)] \\
&= \mathrm{Var}[Y] + \mathrm{Var}[\hat{f}(x_0)] + (f(x_0) - \mathrm{E}[\hat{f}(x_0)])^2 \\
&= \mathrm{Var}(\varepsilon) + \mathrm{Var}[\hat{f}(x_0)] + [\mathrm{Bias}(\hat{f}(x_0))]^2.
\end{aligned}$$

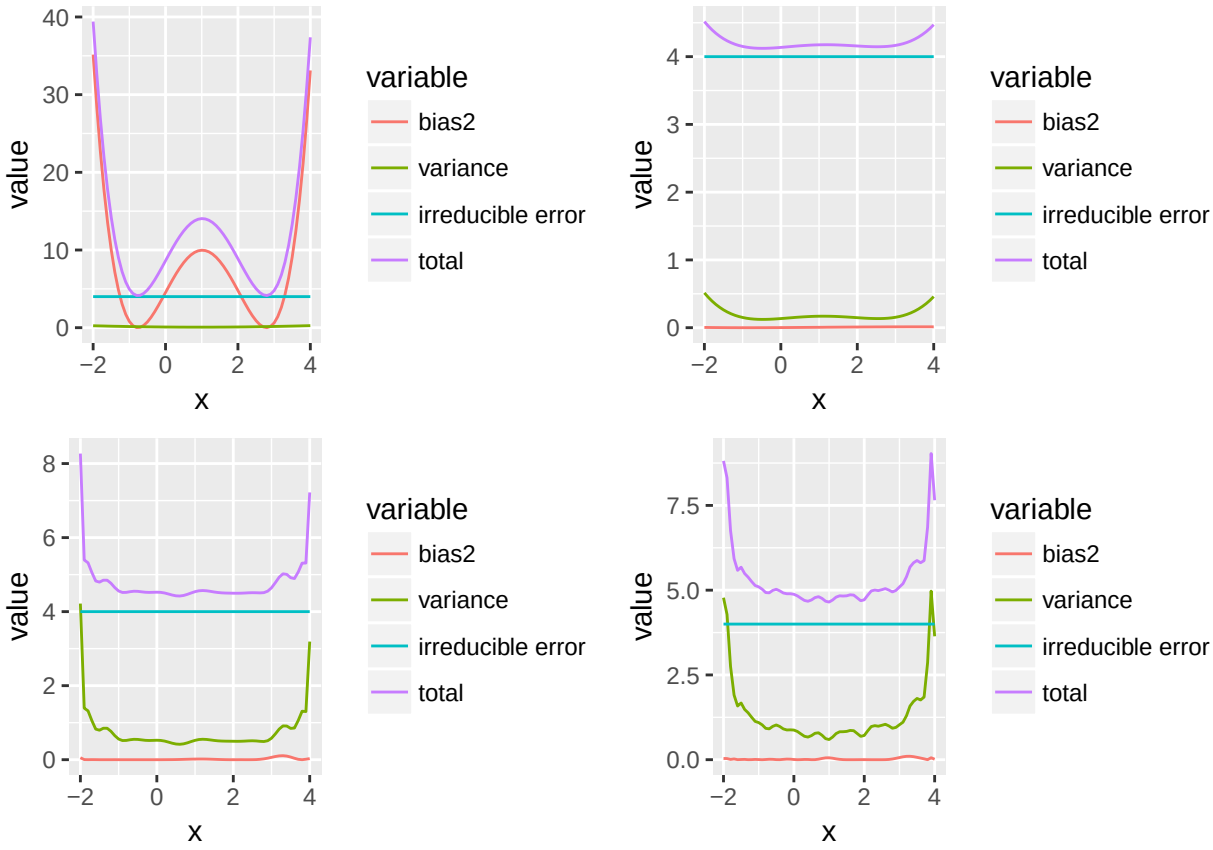
$$\mathrm{E}[(Y - \hat{f}(x_0))^2] = \cdots = \mathrm{Var}(\varepsilon) + \mathrm{Var}[\hat{f}(x_0)] + [\mathrm{Bias}(\hat{f}(x_0))]^2$$

- First term: irreducible error, σ_ε^2 and is always present unless we have measurements without error. This term cannot be reduced regardless how well our statistical model fits the data.
- Second term: variance of the prediction at x_0 or the expected deviation around the mean at x_0. If the variance is high, there is large uncertainty associated with the prediction.
- Third term: squared bias. The bias gives an estimate of how much the prediction differs from the true mean. If the bias is low the model gives a prediction which is close to the true value.

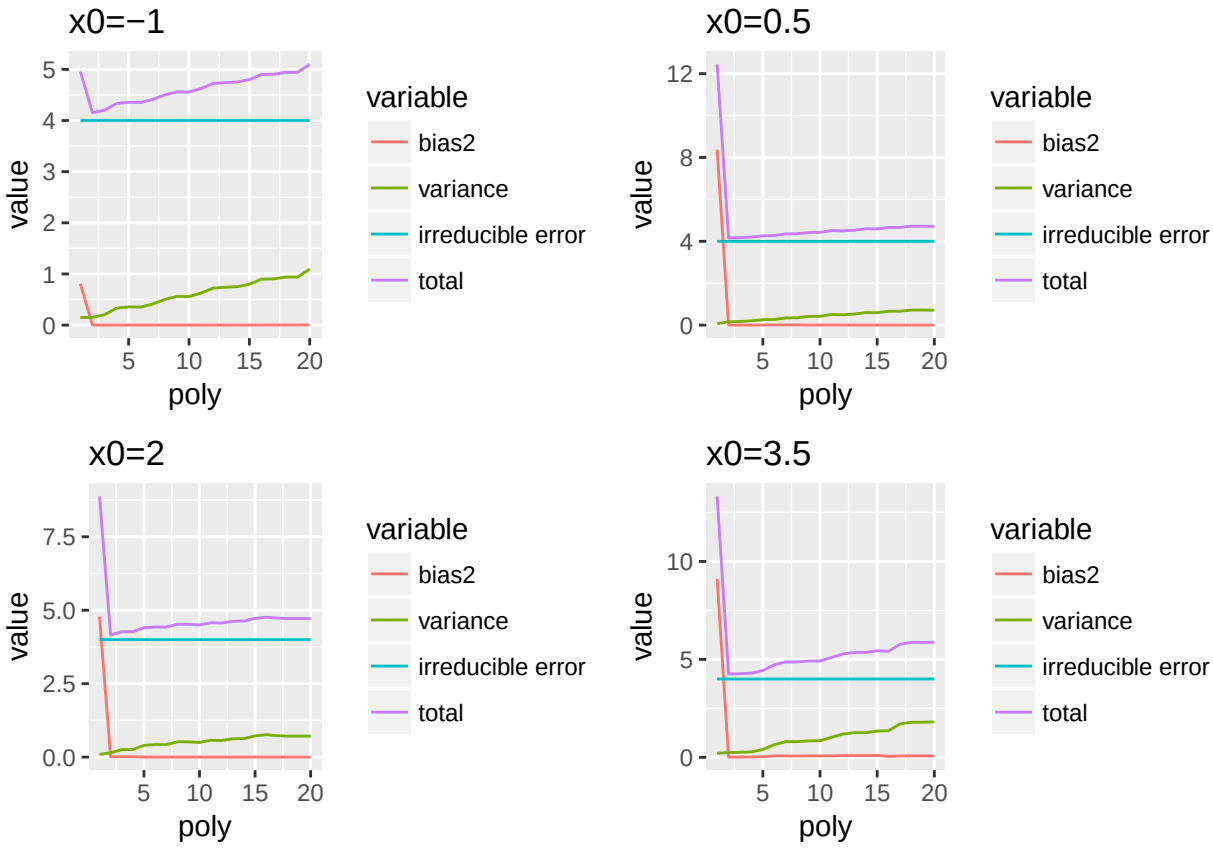
$$\mathrm{E}[(Y - \hat{f}(x_0))^2] = \cdots = \mathrm{Var}(\varepsilon) + \mathrm{Var}[\hat{f}(x_0)] + [\mathrm{Bias}(\hat{f}(x_0))]^2$$

This is the expected test MSE: the average test MSE we would obtain if we repeatedly estimated f using many training sets (as we did in our example), and then tested this estimate at x_0.

The *overall* expected test MSE can we then compute by averaging the expected test MSE at x_0 over all possible values of x_0 (averaging with respect to frequency in test set).



For 4 different polynomial models (poly1,2,10 and 20), the the squared bias, variance, irreducible error and the total sum. Plot based on 100 simulations for the polynomial example.



At 4 different values for x_0, the squared bias, variance, irreducible error and the total sum. Plot based on 100 simulations for the polynomial example.

When fitting a statistical model the aim is often to obtain the most predictive model. There are often many candidate models, and the task is to decide which model to choose.

- The observations used to fit the statistical model make up the training set. The training error is the average loss over the training sample.
- As the complexity (and thus flexibility) of a model increases the model becomes more adaptive to underlying structures and the training error falls.
- However, the variance of will increase (remember variability of order 20 curve).
- This means that new observations will be predicted with a higher uncertainty.
- The test error is the prediction error over a test sample.
- The test sample will have new observations which were not used when fitting the model. One wants the model to capture important relationships between the response variable and the covariates, else we will underfit. Recall the red line in the figure corresponding to the toy example above.

This trade-off in selecting a model with the right amount of complexity/flexibility is the variance-bias trade-off.

We will in Module 8 see how methods as bagging, boosting and random forests can lower the variance while prevailing a low bias.

Classification

(so far, regression setting - but how about model accuracy in classification?)

Set-up: Training observations (independent pairs) $\{(x_1, y_1), ..., (x_n, y_n)\}$ where the response variable Y is qualitative. E.g $Y \in \mathcal{C} = \{0, 1, ..., 9\}$ or $Y \in \mathcal{C} = \{dog, cat, ..., horse\}$.

Aim: To *build* a classifier $f(x)$ that assigns a class label from $\mathcal{C}$ to a future unlabelled observation x and to asses the *uncertainty* in this classification. Sometimes the role of the different predictors may be of main interest.

Performance measure: Most popular is the misclassification error rate (training and test version).

0/1-loss: The misclassifications are given the loss 1 and the correct classifications loss 0. (Quadratic loss is not used for classification.)

Q: Give an example of a classification problem.

Synthetic example

- The figure below shows a plot of 100 observations from two classes A (red dots) and B (turquoise dots),
- simulated from a bivariate normal distribution with mean vectors $\mu_A = (1, 1)^T$ and $\mu_B = (3, 3)^T$ and a covariance matrix $\Sigma_A = \Sigma_B = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$.
- We want to find a rule to classify a new observation to class A or B.

Training error rate

the proportion of mistakes that are made if we apply our estimator $\hat{f}$ to the training observations, i.e. $\hat{y}_i = \hat{f}(x_i)$.

$$\frac{1}{n}\sum_{i=1}^{n} \mathrm{I}(y_i \neq \hat{y}_i).$$

Here I is the indicator function (to give our 0/1 loss) which is defined as:

$$\mathrm{I}(a = \hat{a}) = \begin{cases} 1 \text{ if } a = \hat{a} \\ 0 \text{ else} \end{cases}$$

The indicator function counts the number of times our model has made a wrong classification. The training error rate is the fraction of misclassifications made on our training set. A very low training error rate may imply overfitting.

Test error rate

Here the fraction of misclassifications is calculated when our model is applied on a test set. From what we have learned about regression we can deduct that this gives a better indication of the true performance of the classifier (than the traning error).

$$\mathrm{Ave}(I(y_0 \neq \hat{y}_0))$$

where the average is over all the test observations (x_0, y_0).

We assume that a *good* classifier is a classifier that has a *low* test error.

Bayes classifier

Suppose we have a quantitative response value that can be a member in one of K classes $\mathcal{C} = \{c_1, c_2, ..., c_k, ..., c_K\}$. Further, suppose these elements are numbered $1, 2, ..., K$. The probability of that a new observation x_0 belongs to class k is

$$p_k(x_0) = \Pr(Y = k | X = x_0), \quad k = 1, 2, ...K.$$

This is the conditional class probability: the probability that $Y = k$ given the observation x_0. The *Bayes classifier assigns an observation to the most likely class*, given its predictor values.

This is best illustrated by a two-class example. Assume our response value is to classified as belonging to one of the two groups $\{A, B\}$. A new observation x_0 will be classified to A if $\Pr(Y = A | X = x_0) > 0.5$ and to class B otherwise.

The Bayes classifier

- has the *smallest test error rate.*
- However, we do never know the conditional distribution of Y given X for real data. Computing the Bayes classifier is thus impossible.
- The class boundaries using the Bayes classifier is called the *Bayes decision boundary.*

- The overall Bayes error rate is given as

$$1 - \mathrm{E}(\max \Pr(Y = j \mid X))$$

  where the expectation is over X.
- The Bayes error rate is comparable to the *irreducible error* in the regression setting.

Next: K-nearest neighbor classifier estimates this conditional distribution and then classifies a new observation based on this estimated probability.

K-nearest neighbour classifier

The K-nearest neighbour classifier (KNN) works in the following way:

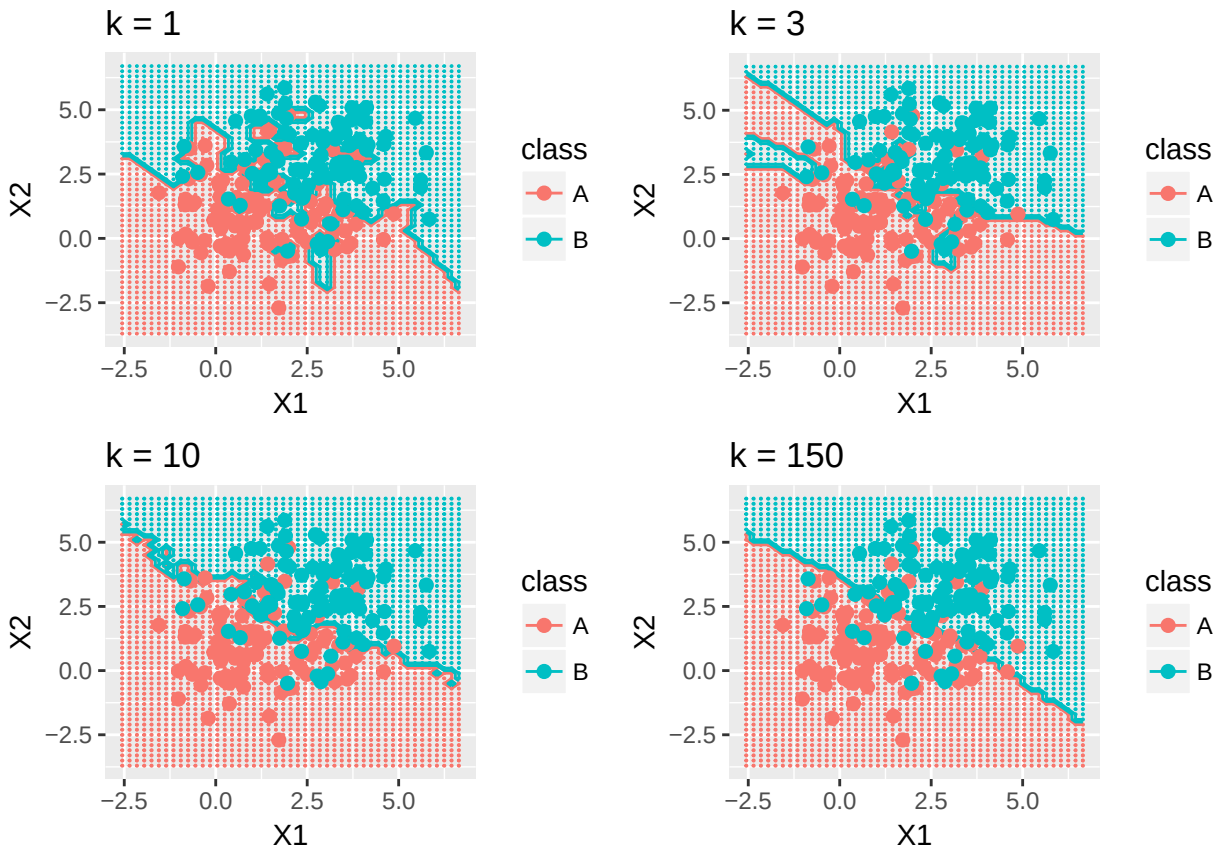
- Given a new observation x_0 it searches for the K points in our training data that are closest to it.
- These points make up the neighborhood of x_0, $\mathcal{N}_0$.
- The point x_0 is classified by taking a majority vote of the neighbors.
- That means that x_0 is classified to the most occurring class among its neighbors

$$\Pr(Y = j | X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j).$$

We return to our synthetic data with X_1 and X_2 and two classes A and V:

- Assume we have a new observation $X_0 = (x_{01}, x_{02})^T$ which we want to classify as belonging to the class A or B.
- To illustrate this problem we fit the K-nearest neighbor classifier to our simulated data set with $K = 1, 3, 10$ and 150 and observe what happens.

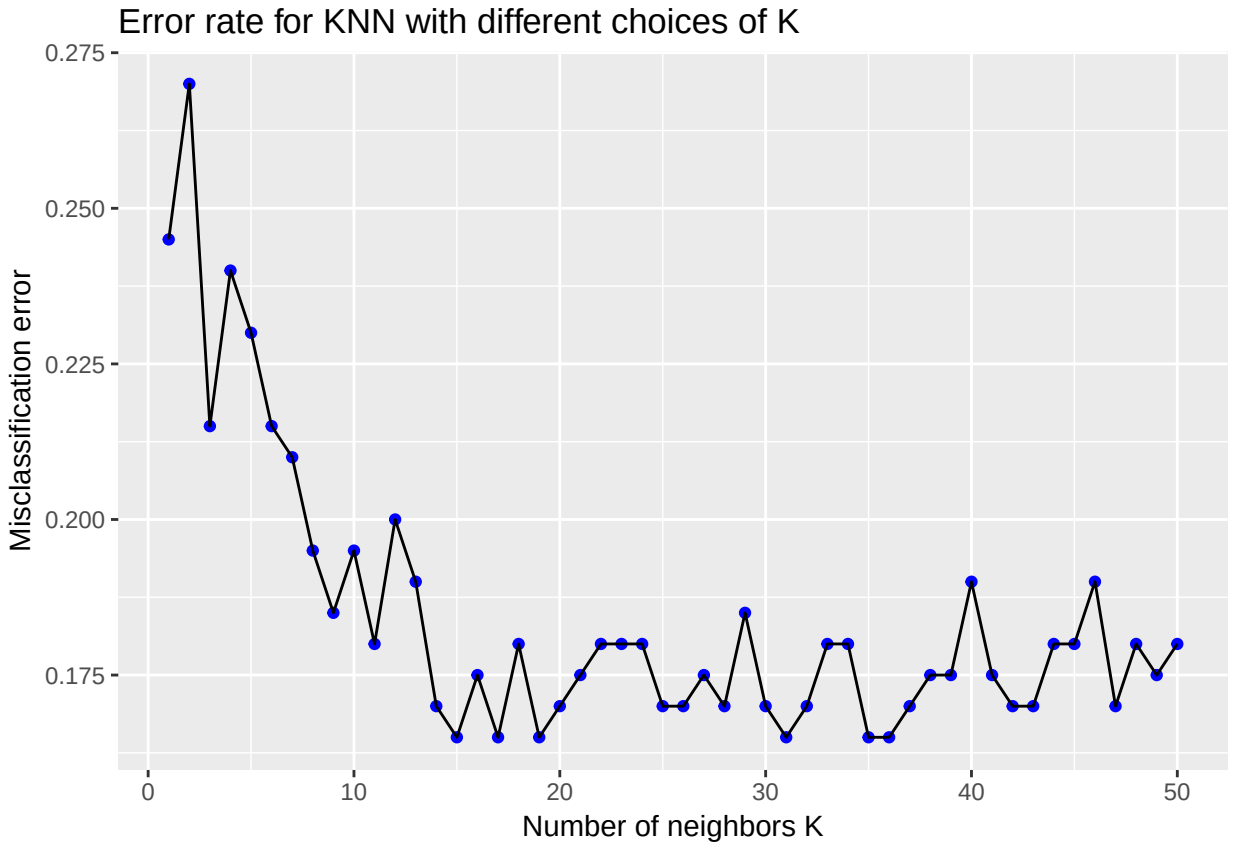
In our plots, the small colored dots show the predicted classes for an evenly-spaced grid. The lines show the decision boundaries. If our new observation falls into the region within the red decision boundary, it will be classified as A. If it falls into the region within the green decision boundary, it will be classified as B.



We see that the choice of K has a big influence on the result of our classification. By choosing $K = 1$ the classification is made to the same class as the one nearest neighbor. When $K = 3$ a majority vote is taken among the three nearest neighbors, and so on. We see that as K gets very large, the decision boundary tends towards a straight line (which is the Bayes boundary in this set-up).

To find the optimal value of K the typical procedure is to try different values of K and then test the predictive power of the different classifiers, for example by cross-validation, which will be discussed in Module 4.

We see that after trying all choices for K between 1 and 50, we see that a few choices of K gave the smallest misclassification error rate, estimating by leave-one out cross-validation (Leave-one-out cross-validation will be discussed in Module 4). The smallest error rate is equal to 0.165. This means that the classifier makes a misclassification 16.5% of the time and a correct classification 83.5% of the time.



This above example showed the bias-variance trade-off in a classification setting. Choosing a value of K amounts to choosing the correct level of flexibility of the classifier. This again is critical to the success of the classifier. A too low value of K will give a very flexible classifier (with high variance and low bias) which will fit the training set too well (it will overfit) and make poor predictions for new observations. Choosing a high value for K makes the classifier loose its flexibility and the classifier will have low variance but high bias.

The curse of dimensionality

The nearest neighbor classifier can be quite good if the number of predictor p is small and the number of observations n is large. We need enough close neighbors to make a good classification.

The effectiveness of the KNN classifier falls quickly when the dimension of the preditor space is high. This is because the nearest neighbors tend to be far away in high dimensions and the method no longer is local. This is referred to as the *curse of dimensionality*.

What was important in Part A?

- prediction vs. interpretation (inference)
- supervised vs. unsupervised methods
- classification vs. regression
- parametric vs. non-parametric methods

- flexibility vs. interpretation
- under- and overfitting
- quadratic and 0/1 loss functions
- training and test MSE and misclassification error
- bias-variance trade off
- Bayes classifier and KNN-classifier

Part B: random vectors, covariance, mvN

- Random vectors,
- the covariance matrix and
- the multivariate normal distribution

Random vector

- A random vector $\mathbf{X}_{(p\times 1)}$ is a p-dimensional vector of random variables.
  - Weight of cork deposits in $p = 4$ directions (N, E, S, W).
  - Rent index in Munich: rent, area, year of construction, location, bath condition, kitchen condition, central heating, district.
- Joint distribution function: $f(\mathbf{x})$.
- From joint distribution function to marginal (and conditional distributions).

$$f_1(x_1) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(x_1, x_2, \ldots, x_p) dx_2 \cdots dx_p$$

- Cumulative distribution (definite integrals!) used to calculate probabilites.
- Independence: $f(x_1, x_2) = f_1(x_1) \cdot f(x_2)$ and $f(x_1 \mid x_2) = f_1(x_1)$.

Moments

The moments are important properties about the distribution of $\mathbf{X}$. We will look at:

- E: Mean of random vector and random matrices.
- Cov: Covariance matrix.
- Corr: Correlation matrix.
- E and Cov of multiple linear combinations.

The Cork deposit data

- Classical multivariate data set from Rao (1948).
- Weigth of bark deposits of $n = 28$ cork trees in $p = 4$ directions (N, E, S, W).

```
corkds=as.matrix(read.table("https://www.math.ntnu.no/emner/TMA4268/2018v/data/corkMKB.txt"))
dimnames(corkds)[[2]]=c("N","E","S","W")
head(corkds)
```

```
##       N  E  S  W
## [1,] 72 66 76 77
## [2,] 60 53 66 63
## [3,] 56 57 64 58
## [4,] 41 29 36 38
## [5,] 32 32 35 36
## [6,] 30 35 34 26
```

Q: How may we define a random vector and random matrix for cork trees?

A: Draw a random sample of size $n = 28$ from the population of cork trees and observe a $p = 4$ dimensional random vector for each tree.

$$\mathbf{X}_{(28\times 4)} = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} \\ X_{21} & X_{22} & X_{23} & X_{24} \\ X_{31} & X_{32} & X_{33} & X_{34} \\ \vdots & \vdots & \ddots & \vdots \\ X_{28,1} & X_{28,2} & X_{28,3} & X_{28,4} \end{bmatrix}$$

Rules for means

- Random vector $\mathbf{X}_{(p\times 1)}$ with mean vector $\mu_{(p\times 1)}$:

$$\mathbf{X}_{(p\times 1)} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{bmatrix}, \text{ and } \mu_{(p\times 1)} = \mathrm{E}(\mathbf{X}) = \begin{bmatrix} \mathrm{E}(X_1) \\ \mathrm{E}(X_2) \\ \vdots \\ \mathrm{E}(X_p) \end{bmatrix}$$

Remark: observe that $\mathrm{E}(X_j)$ is calculated from the marginal distribution of X_j and contains no information about dependencies between X_j and X_k, $k \neq j$.

- Random matrix $\mathbf{X}_{(n\times p)}$ and random matrix $\mathbf{Y}_{(n\times p)}$:

$$\mathrm{E}(\mathbf{X} + \mathbf{Y}) = \mathrm{E}(\mathbf{X}) + \mathrm{E}(\mathbf{Y})$$

Proof: Look at element $Z_{ij} = X_{ij} + Y_{ij}$ and see that $\mathrm{E}(Z_{ij}) = \mathrm{E}(X_{ij} + Y_{ij}) = \mathrm{E}(X_{ij}) + \mathrm{E}(Y_{ij})$.

- Random matrix $\mathbf{X}_{(n\times p)}$ and conformable constant matrices $\mathbf{A}$ and $\mathbf{B}$:

$$\mathrm{E}(\mathbf{AXB}) = \mathbf{A}\mathrm{E}(\mathbf{X})\mathbf{B}$$

Proof: Look at element (i, j) of $\mathbf{AXB}$

$$e_{ij} = \sum_{k=1}^{n} a_{ik} \sum_{l=1}^{p} X_{kl} b_{lj}$$

(where a_{ik} and b_{lj} are elements of $\mathbf{A}$ and $\mathbf{B}$ respectively), and see that $\mathrm{E}(e_{ij})$ is the element (i, j) if $\mathbf{A}\mathrm{E}(\mathbf{X})\mathbf{B}$.

Q: what are the univariate analog to this formula - that you studied in your first introductory course in statistics? What do you think happens if we look at $\mathrm{E}(\mathbf{AXB}) + \mathbf{d}$?

A: $ ext{E}(aX+b)=a ext{E}(X)+b$

Variance-covariance matrix

Q: In the introductory statistics course we define the the covariance $\text{Cov}(X_i, X_j) = \text{E}[(X_i - \mu_i)(X_j - \mu_j)] = \text{E}(X_i \cdot X_j) - \mu_i \mu_j$.

- What is the covariance called when $i = j$?
- What does it mean when the covariance is
  - negative
  - zero
  - positive?

- Consider random vector $\mathbf{X}_{(p\times 1)}$ with mean vector $\mu_{(p\times 1)}$:

$$\mathbf{X}_{(p\times 1)} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{bmatrix}, \text{ and } \mu_{(p\times 1)} = \text{E}(\mathbf{X}) = \begin{bmatrix} \text{E}(X_1) \\ \text{E}(X_2) \\ \vdots \\ \text{E}(X_p) \end{bmatrix}$$

- Variance-covariance matrix Σ (real and symmetric)

$$\Sigma = \text{Cov}(\mathbf{X}) = \text{E}[(\mathbf{X} - \mu)(\mathbf{X} - \mu)^T] = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_{pp} \end{bmatrix} = \text{E}(\mathbf{X}\mathbf{X}^T) - \mu\mu^T$$

- Elements: $\sigma_{ij} = \text{E}[(X_i - \mu_i)(X_j - \mu_j)] = \sigma_{ji}$.

Remark: the matrix Σ is called variance, covariance and variance-covariance matrix and denoted both $\text{Var}(\mathbf{X})$ and $\text{Cov}(\mathbf{X})$.

Remark: observe the notation of elements $\sigma_{11} = \sigma_1^2$ is a variance.

Exercise: the variance-covariance matrix

Let $\mathbf{X}_{4\times 1}$ have variance-covariance matrix

$$\Sigma = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix}.$$

Explain what this means.

Correlation matrix

Correlation matrix ρ (real and symmetric)

$$\rho = \begin{bmatrix} \frac{\sigma_{11}}{\sqrt{\sigma_{11}\sigma_{11}}} & \frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}} & \cdots & \frac{\sigma_{1p}}{\sqrt{\sigma_{11}\sigma_{pp}}} \\ \frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}} & \frac{\sigma_{22}}{\sqrt{\sigma_{22}\sigma_{22}}} & \cdots & \frac{\sigma_{2p}}{\sqrt{\sigma_{22}\sigma_{pp}}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sigma_{1p}}{\sqrt{\sigma_{11}\sigma_{pp}}} & \frac{\sigma_{2p}}{\sqrt{\sigma_{22}\sigma_{pp}}} & \cdots & \frac{\sigma_{pp}}{\sqrt{\sigma_{pp}\sigma_{pp}}} \end{bmatrix} = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{12} & 1 & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1p} & \rho_{2p} & \cdots & 1 \end{bmatrix}$$

$$\rho = (\mathbf{V}^{\frac{1}{2}})^{-1}\Sigma(\mathbf{V}^{\frac{1}{2}})^{-1}, \text{ where } \mathbf{V}^{\frac{1}{2}} = \begin{bmatrix} \sqrt{\sigma_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{\sigma_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\sigma_{pp}} \end{bmatrix}$$

Exercise: the correlation matrix

Let $\mathbf{X}_{4\times 1}$ have variance-covariance matrix

$$\Sigma = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix}.$$

Find the correlation matrix.

A:

$$\rho = \begin{bmatrix} 1 & 0.5 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0.5 \\ 0 & 0 & 1 & 0.5 \\ 0 & 0.5 & 0.5 & 1 \end{bmatrix}$$

Linear combinations

Consider a random vector $\mathbf{X}_{(p\times 1)}$ with mean vector $\mu = \mathrm{E}(\mathbf{X})$ and variance-covariance matrix $\Sigma = \mathrm{Cov}(\mathbf{X})$.

The linear combinations

$$\mathbf{Z} = \mathbf{C}\mathbf{X} = \begin{bmatrix} \sum_{j=1}^{p} c_{1j}X_j \\ \sum_{j=1}^{p} c_{2j}X_j \\ \vdots \\ \sum_{j=1}^{p} c_{kj}X_j \end{bmatrix}$$

have

$$\mathrm{E}(\mathbf{Z}) = \mathrm{E}(\mathbf{C}\mathbf{X}) = \mathbf{C}\mu$$
$$\mathrm{Cov}(\mathbf{Z}) = \mathrm{Cov}(\mathbf{C}\mathbf{X}) = \mathbf{C}\Sigma\mathbf{C}^T$$

Proof

Exercise: Study the proof - what are the most important transitions?

Exercise: Linear combinations

$$\mathbf{X} = \begin{bmatrix} X_N \\ X_E \\ X_S \\ X_W \end{bmatrix}, \text{ and } \mu = \begin{bmatrix} \mu_N \\ \mu_E \\ \mu_S \\ \mu_W \end{bmatrix}, \text{ and } \Sigma = \begin{bmatrix} \sigma_{NN} & \sigma_{NE} & \sigma_{NS} & \sigma_{NW} \\ \sigma_{NE} & \sigma_{EE} & \sigma_{ES} & \sigma_{EW} \\ \sigma_{NS} & \sigma_{EE} & \sigma_{SS} & \sigma_{SW} \\ \sigma_{NW} & \sigma_{EW} & \sigma_{SW} & \sigma_{WW} \end{bmatrix}$$

Scientists would like to compare the following three *contrasts*: N-S, E-W and (E+W)-(N+S), and define a new random vector $\mathbf{Y}_{(3\times1)} = \mathbf{C}_{(3\times4)}\mathbf{X}_{(4\times1)}$ giving the three contrasts.

- Write down $\mathbf{C}$.
- Explain how to find $\mathrm{E}(Y_1)$ and $\mathrm{Cov}(Y_1, Y_3)$.
- Use R to find the mean vector, covariance matrix and correlations matrix of $\mathbf{Y}$, when the mean vector and covariance matrix for $\mathbf{X}$ is given below.

```
corkds <- as.matrix(read.table("https://www.math.ntnu.no/emner/TMA4268/2018v/data/corkMKB.txt"))
dimnames(corkds)[[2]] <- c("N","E","S","W")
mu=apply(corkds,2,mean)
mu
Sigma=var(corkds)
Sigma
```

```
##        N        E        S        W
## 50.53571 46.17857 49.67857 45.17857
##          N        E        S        W
## N 290.4061 223.7526 288.4378 226.2712
## E 223.7526 219.9299 229.0595 171.3743
## S 288.4378 229.0595 350.0040 259.5410
## W 226.2712 171.3743 259.5410 226.0040
```

The covariance matrix - more requirements?

Random vector $\mathbf{X}_{(p\times1)}$ with mean vector $\mu_{(p\times1)}$ and covariance matrix

$$\Sigma = \mathrm{Cov}(\mathbf{X}) = \mathrm{E}[(\mathbf{X}-\mu)(\mathbf{X}-\mu)^T] = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_{pp} \end{bmatrix}$$

The covariance matrix is by construction symmetric, and it is common to require that the covariance matrix is positive definite. Why do you think that is?

Hint: What is the definition of a positive definite matrix? Is it possible that the variance of the linear combination $\mathbf{Y} = \mathbf{c}^T\mathbf{X}$ is negative?

Multiple choice - random vectors

Choose the correct answer - time limit was 30 seconds for each question! Let's go!

Mean of sum

$\mathbf{X}$ and $\mathbf{Y}$ are two bivariate random vectors with $\mathrm{E}(\mathbf{X}) = (1, 2)^T$ and $\mathrm{E}(\mathbf{Y}) = (2, 0)^T$. What is $\mathrm{E}(\mathbf{X} + \mathbf{Y})$?

- A: $(1.5, 1)^T$
- B: $(3, 2)^T$
- C: $(-1, 2)^T$
- D: $(1, -2)^T$

Mean of linear combination

$\mathbf{X}$ is a 2-dimensional random vector with $\mathrm{E}(\mathbf{X}) = (2, 5)^T$, and $\mathbf{b} = (0.5, 0.5)^T$ is a constant vector. What is $\mathrm{E}(\mathbf{b}^T\mathbf{X})$?

- A: 3.5
- B: 7
- C: 2
- D: 5

Covariance

$\mathbf{X}$ is a p-dimensional random vector with mean μ. Which of the following defines the covariance matrix?

- A: $E[(\mathbf{X} - \mu)^T(\mathbf{X} - \mu)]$
- B: $E[(\mathbf{X} - \mu)(\mathbf{X} - \mu)^T]$
- C: $E[(\mathbf{X} - \mu)(\mathbf{X} - \mu)]$
- D: $E[(\mathbf{X} - \mu)^T(\mathbf{X} - \mu)^T]$

Mean of linear combinations

$\mathbf{X}$ is a p-dimensional random vector with mean μ and covariance matrix Σ. $\mathbf{C}$ is a constant matrix. What is then the mean of the k-dimensional random vector $\mathbf{Y} = \mathbf{C}\mathbf{X}$?

- A: $\mathbf{C}\mu$
- B: $\mathbf{C}\Sigma$
- C: $\mathbf{C}\mu\mathbf{C}^T$
- D: $\mathbf{C}\Sigma\mathbf{C}^T$

Covariance of linear combinations

$\mathbf{X}$ is a p-dimensional random vector with mean μ and covariance matrix Σ. $\mathbf{C}$ is a constant matrix. What is then the covariance of the k-dimensional random vector $\mathbf{Y} = \mathbf{C}\mathbf{X}$?

- A: $\mathbf{C}\mu$
- B: $\mathbf{C}\Sigma$
- C: $\mathbf{C}\mu\mathbf{C}^T$

- D: $\mathbf{C}\Sigma\mathbf{C}^T$

Correlation

$\mathbf{X}$ is a 2-dimensional random vector with covariance matrix

$$\Sigma = \begin{bmatrix} 4 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$

Then the correlation between the two elements of $\mathbf{X}$ are:

- A: 0.10
- B: 0.25
- C: 0.40
- D: 0.80

Answers:

BABADC

The multivariate normal distribution

Why is the mvN so popular?

- Many natural phenomena may be modelled using this distribution (just as in the univariate case).
- Multivariate version of the central limit theorem- the sample mean will be approximately multivariate normal for large samples.
- Good interpretability of the covariance.
- Mathematically tractable.
- Building block in many models and methods.

Suggested reading (if you want to know more than you learn here): Härdle and Simes (2015): Chapter 4.4 and 5.1 (ebook free for NTNU students) (on the reading list for TMA4267 Linear statistical models).

See the 3D-printed mvNs in class!

The multivariate normal (mvN) pdf

The random vector $\mathbf{X}_{p\times 1}$ is multivariate normal N_p with mean μ and (positive definite) covariate matrix Σ. The pdf is:

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{p}{2}}|\Sigma|^{\frac{1}{2}}} \exp\{-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)\}$$

Q:

- How does this compare to the univariate version?

$$f(x) = \frac{1}{2\sqrt{\pi}\sigma} \exp\{\frac{1}{2\sigma^2}(x-\mu)^2\}$$

- Why do we need the constant in front of the exp?
- What is the dimension of the part in exp? (This is a quadratic form, a central topic in TMA4267.)

Six useful properties of the mvN

Let $\mathbf{X}_{(p\times 1)}$ be a random vector from $N_p(\mu, \Sigma)$.

1. The grapical contours of the mvN are ellipsoids (can be shown using spectral decomposition).
2. Linear combinations of components of $\mathbf{X}$ are (multivariate) normal (can be easily proven using moment generating functions MGF).
3. All subsets of the components of $\mathbf{X}$ are (multivariate) normal (special case of the above).
4. Zero covariance implies that the corresponding components are independently distributed (can be proven using MGF).
5. $\mathbf{A}\Sigma\mathbf{B}^T = \mathbf{0} \Leftrightarrow \mathbf{AX}$ and $\mathbf{BX}$ are independent.
6. The conditional distributions of the components are (multivariate) normal.

$$\mathbf{X}_2 \mid (\mathbf{X}_1 = \mathbf{x}_1) \sim N_{p2}(\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}).$$

All of these are proven in TMA4267 Linear Statistical Models (mainly using moment generating functions).

The result 4 is rather useful! If you have a bivariate normal and observed covariance 0, then your variables are independent.

Contours of multivariate normal distribution

Contours of constant density for the p-dimensional normal distribution are ellipsoids defined by $\mathbf{x}$ such that

$$(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu) = b$$

where $b > 0$ is a constant.

These ellipsoids are centered at μ and have axes $\pm\sqrt{b\lambda_i}\mathbf{e}_i$, where $\Sigma\mathbf{e}_i = \lambda_i\mathbf{e}_i$, for $i = 1, ..., p$.

Remark: to see this the spectral decomposition of the covariance matrix is useful.

- $(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)$ is distributed as χ^2_p.
- The volume inside the ellipsoid of $\mathbf{x}$ values satisfying

  $$(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu) \leq \chi^2_p(\alpha)$$

  has probability $1-\alpha$.

In Module 4: Classification the mvN is very important and we will often draw contours of the mvN as ellipses- and this is the reason why.

Q: Take a look at the 3D-printed figures - there you may see that with equal variances we have circles and with unequal variances we have ellipses.

Identify the 3D-printed mvNs

Let $\Sigma = \begin{bmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{bmatrix}$.

The following four 3D-printed figures have been made:

- A: $\sigma_x = 1$, $\sigma_y = 2$, $\rho = 0.3$
- B: $\sigma_x = 1$, $\sigma_y = 1$, $\rho = 0$
- C: $\sigma_x = 1$, $\sigma_y = 1$, $\rho = 0.5$
- D: $\sigma_x = 1$, $\sigma_y = 2$, $\rho = 0$

The figures have the following colours:

- white
- purple
- red
- black

Task: match letter and colour.

Answers: A black, B purple, C red and D white

Multiple choice - multivariate normal

Choose the correct answer - time limit was 30 seconds for each question! Let's go!

Multivariate normal pdf

The probability density function is $(\frac{1}{2\pi})^{\frac{p}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\{-\frac{1}{2}Q\}$ where Q is

- A: $(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)$
- B: $(\mathbf{x}-\mu)\Sigma(\mathbf{x}-\mu)^T$
- C: $\Sigma - \mu$

Trivariate normal pdf

What graphical form has the solution to $f(\mathbf{x}) =$ constant?

- A: Circle
- B: Parabola
- C: Ellipsoid
- D: Bell shape

Multivariate normal distribution

$\mathbf{X}_p \sim N_p(\mu, \Sigma)$, and $\mathbf{C}$ is a $k \times p$ constant matrix. $\mathbf{Y} = \mathbf{CX}$ is

- A: Chi-squared with k degrees of freedom
- B: Multivariate normal with mean $k\mu$
- C: Chi-squared with p degrees of freedom

- D: Multivariate normal with mean $\mathbf{C}\mu$

Independence

Let $\mathbf{X} \sim N_3(\mu, \Sigma)$, with

$$\Sigma = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 3 & 2 \\ 0 & 2 & 5 \end{bmatrix}.$$

Which two variables are independent?

- A: X_1 and X_2
- B: X_1 and X_3
- C: X_2 and X_3
- D: None – but two are uncorrelated.

Constructing independent variables?

Let $\mathbf{X} \sim N_p(\mu, \Sigma)$. How can I construct a vector of independent standard normal variables from $\mathbf{X}$?

- A: $\Sigma(\mathbf{X} - \mu)$
- B: $\Sigma^{-1}(\mathbf{X} + \mu)$
- C: $\Sigma^{-\frac{1}{2}}(\mathbf{X} - \mu)$
- D: $\Sigma^{\frac{1}{2}}(\mathbf{X} + \mu)$

Conditional distribution: mean

$\mathbf{X} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ is a bivariate normal random vector. What is true for the conditional mean of $\backslash X_2$ given $X_1 = x_1$?

- A: Not a function of x_1
- B: A linear function of x_1
- C: A quadratic function of x_1

Conditional distribution: variance

$\mathbf{X} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ is a bivariate normal random vector. What is true for the conditional variance of X_2 given $X_1 = x_1$?

- A: Not a function of x_1
- B: A linear function of x_1
- C: A quadratic function of x_1

Answers:

ACDBCBA

Recommended exercises

Problem 1: Reflections and practicals

1. Describe a real-life application in which classification might be useful. Identify the response and the predictors. Is the goal inference or prediction?
2. Describe a real-life application in which regression might be useful. Identify the response and the predictors. Is the goal inference or prediction?
3. Take a look at Figure 2.9 in the book (p. 31).
    a. Will a flexible or rigid method typically have the highest test error?
    b. Does a small variance imply an overfit or rather an underfit to the data?
    c. Relate the problem of over-and underfitting to the bias-variance trade-off.
4. Exercise 7 from the book (p.53) slightly modified. The table below provides a training data set consisting of seven observations, two predictors and one qualitative response variable.

```
library(knitr)
library(kableExtra)
knnframe = data.frame(x1 = c(3, 2, 1, 0, -1, 2, 1), x2 = c(3, 0, 1, 1, 0, 1, 0),  y=c("A", "A", "A", "B
#kable(knnframe,format="html")
kable(knnframe)
```

x1	x2	y
3	3	A
2	0	A
1	1	A
0	1	B
-1	0	B
2	1	B
1	0	B

We wish to use this data set to make a prediction for Y when $X_1 = 1, X_2 = 2$ using the K-nearest neighbors classification method.

a. Compute the Euclidean distance between each observation and the test point, $X_1 = 1, X_2 = 2$.
b. What is our prediction with $K = 1$? Why?
c. What is our prediction with $K = 4$? Why?
d. If the Bayes decision boundary in this problem is highly non-linear, when would we expect the best value for K to be large or small? Why?
e. Install and load the `ggplot2` library:

```
install.packages(ggplot2)
library(ggplot2)
```

Plot the points in `R` using the functions `ggplot`, and `geom_points`.

f. Use the function `knn` from the `class` library to make a prediction for the test point using `k=1`. Do you obtain the same result as by hand?
g. Use the function `knn` to make a prediction for the test point using `k=4` and `k=7`.

Problem 2: Theory and practice - MSEtrain, MSEtest, and bias-variance

We will now look closely into the simulations and calculations performed for the MSEtrain, MSEtest, and bias-variance trade-off in PartA.

- The simulations are based on $f(x) = x^2$ and normal noise with mean 0 and standard deviation 2 is added.
- x is on a 0.1 grid from -2 to 4.
- Parametric models of different complexity are fitted - poly1-poly2
- M=100 simulations are done.

The aim of this problem is to understand:

- trainMSE
- testMSE
- bias-variance trade-off

---

a) Problem set-up

- See the code below. Explain what is done. (You need not understand the code in detail.) Run the code.
- We will learn more about the `lm` function in Module 3 - now just think of this as fitting a polynomial regression and predict gives the fitted curve in our grid points. `predarray` is just a way to save M simulations of 61 gridpoints in x and 20 polynomial models.

```
library(ggplot2)
library(ggpubr)
set.seed(2) # to reproduce

M=100 # repeated samplings, x fixed
nord=20 # order of polynoms


x = seq(-2, 4, 0.1)
truefunc=function(x) return(x^2)
true_y = truefunc(x)

error = matrix(rnorm(length(x)*M, mean=0, sd=2),nrow=M,byrow=TRUE)
ymat = matrix(rep(true_y,M),byrow=T,nrow=M) + error

predarray=array(NA,dim=c(M,length(x),nord))
for (i in 1:M)
{
  for (j in 1:nord)
  {
    predarray[i,,j]=predict(lm(ymat[i,]~poly(x,j,raw=TRUE)))
  }
}
```

```r
# M matrices of size length(x) times nord
# first, only look at variablity in the M fits and plot M curves where we had 1

# for plotting need to stack the matrices underneath eachother and make new variable "rep"
stackmat=NULL
for (i in 1:M) stackmat=rbind(stackmat,cbind(x,rep(i,length(x)),predarray[i,,]))
#dim(stackmat)
colnames(stackmat)=c("x","rep",paste("poly",1:20,sep=""))
sdf=as.data.frame(stackmat) #NB have poly1-20 now - but first only use 1,2,20
# to add true curve using stat_function - easiest solution
true_x=x
yrange=range(apply(sdf,2,range)[,3:22])
p1=ggplot(data=sdf,aes(x=x,y=poly1,group=rep,colour=rep))+scale_y_continuous(limits=yrange)+geom_line()
p1=p1+stat_function(fun=truefunc,lwd=1.3,colour="black")+ggtitle("poly1")
p2=ggplot(data=sdf,aes(x=x,y=poly2,group=rep,colour=rep))+scale_y_continuous(limits=yrange)+geom_line()
p2=p2+stat_function(fun=truefunc,lwd=1.3,colour="black")+ggtitle("poly2")
p10=ggplot(data=sdf,aes(x=x,y=poly10,group=rep,colour=rep))+scale_y_continuous(limits=yrange)+geom_line
p10=p10+stat_function(fun=truefunc,lwd=1.3,colour="black")+ggtitle("poly10")
p20=ggplot(data=sdf,aes(x=x,y=poly20,group=rep,colour=rep))+scale_y_continuous(limits=yrange)+geom_line
p20=p20+stat_function(fun=truefunc,lwd=1.3,colour="black")+ggtitle("poly20")
ggarrange(p1,p2,p10,p20)
```

---

b) Train and test MSE

- First we produce predictions at each grid point based on our training data (`x` and `ymat`)
- but we also draw new observations to calculate testMSE - see `testymat`
- observe how trainMSE and testMSE is calculated
- run the code

```r
set.seed(2) # to reproduce

M=100 # repeated samplings,x fixed but new errors
nord=20
x = seq(-2, 4, 0.1)
truefunc=function(x) return(x^2)
true_y = truefunc(x)

error = matrix(rnorm(length(x)*M, mean=0, sd=2),nrow=M,byrow=TRUE)
testerror = matrix(rnorm(length(x)*M, mean=0, sd=2),nrow=M,byrow=TRUE)
ymat = matrix(rep(true_y,M),byrow=T,nrow=M) + error
testymat = matrix(rep(true_y,M),byrow=T,nrow=M) + testerror

predarray=array(NA,dim=c(M,length(x),nord))
for (i in 1:M)
{
  for (j in 1:nord)
  {
    predarray[i,,j]=predict(lm(ymat[i,]~poly(x,j,raw=TRUE)))
  }
}
trainMSE=matrix(ncol=nord,nrow=M)
```

```
for (i in 1:M) trainMSE[i,]=apply((predarray[i,,]-ymat[i,])^2,2,mean)
testMSE=matrix(ncol=nord,nrow=M)
for (i in 1:M) testMSE[i,]=apply((predarray[i,,]-testymat[i,])^2,2,mean)
```

- Then we plot train and testMSE - first for one train + test data set, then for 99 more.

```
library(ggplot2)
library(ggpubr)

# format suitable for plotting
stackmat=NULL
for (i in 1:M) stackmat=rbind(stackmat,cbind(rep(i,nord),1:nord,trainMSE[i,],testMSE[i,]))
colnames(stackmat)=c("rep","poly","trainMSE","testMSE")
sdf=as.data.frame(stackmat)
yrange=range(sdf[,3:4])
p1=ggplot(data=sdf[1:nord,],aes(x=poly,y=trainMSE))+scale_y_continuous(limits=yrange)+geom_line()
pall= ggplot(data=sdf,aes(x=poly,group=rep,y=trainMSE,colour=rep))+scale_y_continuous(limits=yrange)+ge
testp1=ggplot(data=sdf[1:nord,],aes(x=poly,y=testMSE))+scale_y_continuous(limits=yrange)+geom_line()
testpall= ggplot(data=sdf,aes(x=poly,group=rep,y=testMSE,colour=rep))+scale_y_continuous(limits=yrange)
ggarrange(p1,pall,testp1,testpall)
```

- More plots: first boxplot and then mean for train and test MSE

```
library(reshape2)
df=melt(sdf,id=c("poly","rep"))[,-2]
colnames(df)[2]="MSEtype"
ggplot(data=df,aes(x=as.factor(poly),y=value))+geom_boxplot(aes(fill=MSEtype))
```

```
trainMSEmean=apply(trainMSE,2,mean)
testMSEmean=apply(testMSE,2,mean)
meandf=melt(data.frame(cbind("poly"=1:nord,trainMSEmean,testMSEmean)),id="poly")
ggplot(data=meandf,aes(x=poly,y=value,colour=variable))+geom_line()
```

---

c) Bias and variance - we use the truth!

Finally, we want to see how the expected quadratic loss can be decomposed into

- irreducible error: $\mathrm{Var}(\varepsilon) = 4$
- squared bias: difference between mean of estimated parametric model chosen and the true underlying curve (`truefunc`)
- variance: variance of the estimated parametric model

Notice that the test data is not used - only predicted values in each x grid point.

Study and run the code. Explain the plots produced.

```
meanmat=matrix(ncol=length(x),nrow=nord)
varmat=matrix(ncol=length(x),nrow=nord)
for (j in 1:nord)
{
  meanmat[j,]=apply(predarray[,,j],2,mean) # we now take the mean over the M simulations - to mimic E a
  varmat[j,]=apply(predarray[,,j],2,var)
}
# nord times length(x)
bias2mat=(meanmat-matrix(rep(true_y,nord),byrow=TRUE,nrow=nord))^2 #here the truth is finally used!
```

- Plotting polys as a function of x

```
df=data.frame(rep(x,each=nord),rep(1:nord,length(x)),c(bias2mat),c(varmat),rep(4,prod(dim(varmat)))) #i
colnames(df)=c("x","poly","bias2","variance","irreducible error") #suitable for plotting
df$total=df$bias2+df$variance+df$`irreducible error`
hdf=melt(df,id=c("x","poly"))
hdf1=hdf[hdf$poly==1,]
hdf2=hdf[hdf$poly==2,]
hdf10=hdf[hdf$poly==10,]
hdf20=hdf[hdf$poly==20,]

p1=ggplot(data=hdf1,aes(x=x,y=value,colour=variable))+geom_line()+ggtitle("poly1")
p2=ggplot(data=hdf2,aes(x=x,y=value,colour=variable))+geom_line()+ggtitle("poly2")
p10=ggplot(data=hdf10,aes(x=x,y=value,colour=variable))+geom_line()+ggtitle("poly10")
p20=ggplot(data=hdf20,aes(x=x,y=value,colour=variable))+geom_line()+ggtitle("poly20")
ggarrange(p1,p2,p10,p20)
```

- Now plotting effect of more complex model at 4 chosen values of x, compare to Figures in 2.12 on page 36 in ISL (our textbook).

```
hdfatxa=hdf[hdf$x==-1,]
hdfatxb=hdf[hdf$x==0.5,]
hdfatxc=hdf[hdf$x==2,]
hdfatxd=hdf[hdf$x==3.5,]
pa=ggplot(data=hdfatxa,aes(x=poly,y=value,colour=variable))+geom_line()+ggtitle("x0=-1")
pb=ggplot(data=hdfatxb,aes(x=poly,y=value,colour=variable))+geom_line()+ggtitle("x0=0.5")
pc=ggplot(data=hdfatxc,aes(x=poly,y=value,colour=variable))+geom_line()+ggtitle("x0=2")
pd=ggplot(data=hdfatxd,aes(x=poly,y=value,colour=variable))+geom_line()+ggtitle("x0=3.5")
ggarrange(pa,pb,pc,pd)
```

---

d) Repeat a-c

- Then try to change the true function `truefunc` to something else - mayby order 3? What does this do the the plots produced? Maybe you then also want to plot poly3?
- Also try to change the standard deviation of the noise added to the curve (now it is sd=2). What happens if you change this to sd=1 or sd=3?
- Or, change to the true function that is not a polynomial?

Problem 3: Visualization tools in R

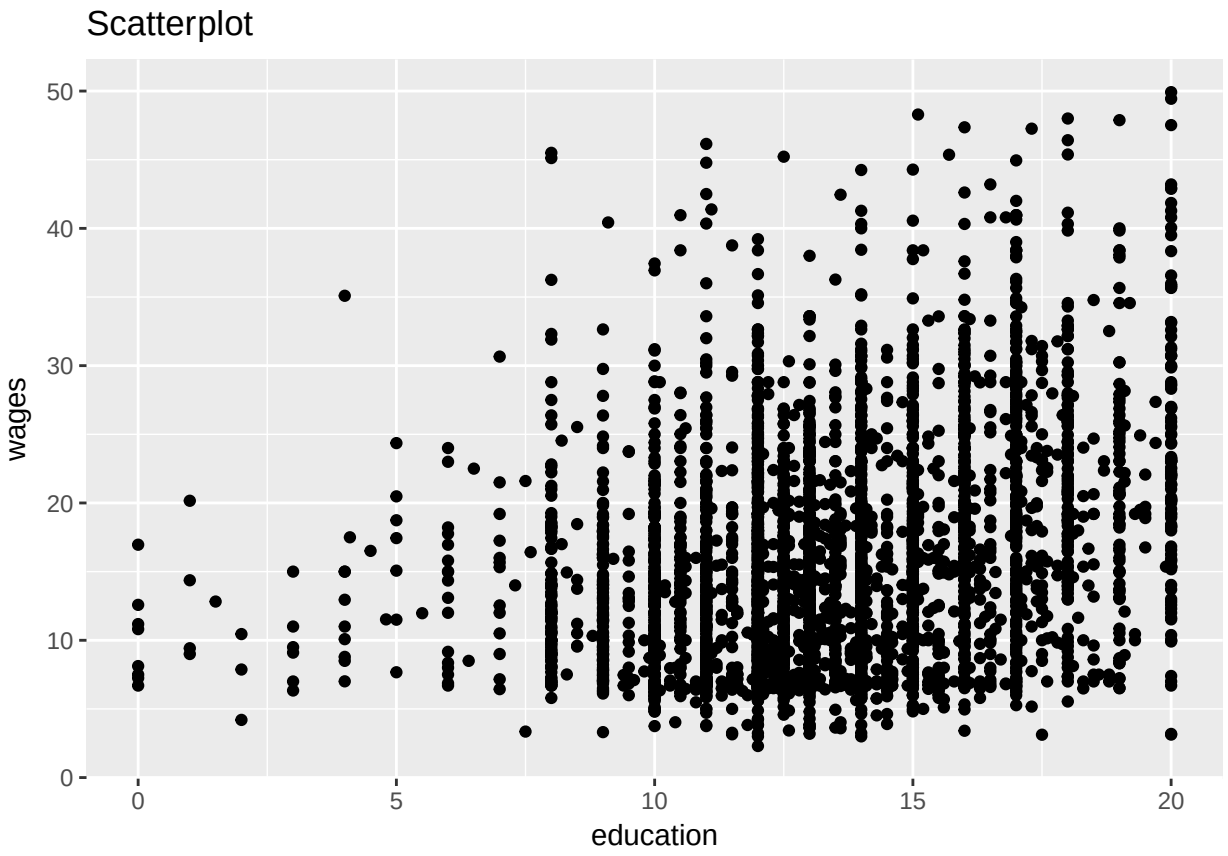
For each of the plots (scatter plot, histogram, boxplot, area chart, heat map, correlogram) *explain what you see (including what is on the x- and y-axis) and try to transform what you see into insight about the data.* All except the correlogram use `ggplot2` for plotting. If you want to read more about the idea behind `ggplot2` (grammar of graphics) Chapter 3 of R for Data Science is a good read.

Three different data sets are used - read descriptions in R:

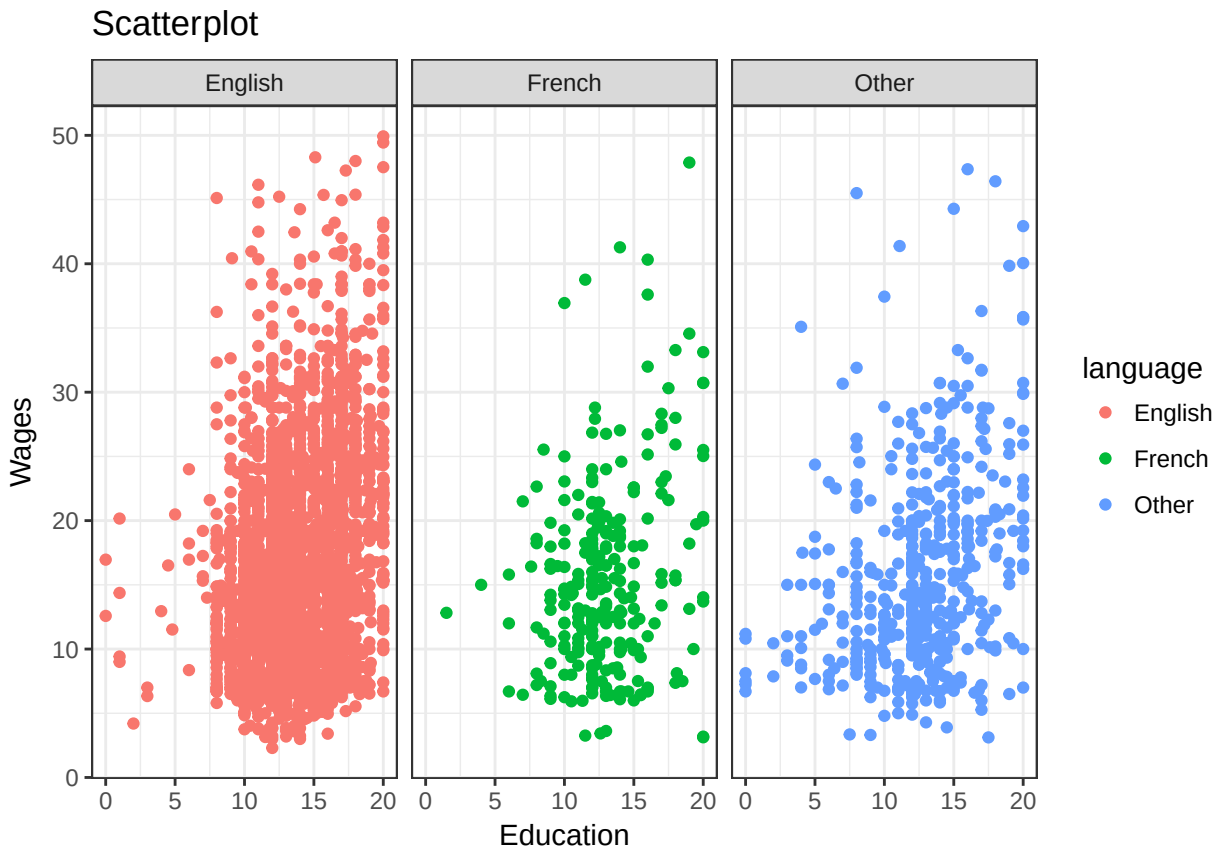
- `SLID`: `?car::SLID`
- `mtcars`: `?datasets::mtcars`
- `ozone`: `?faraway::ozone`

Scatter Plot

```
library(car)
library(ggplot2)
SLID = na.omit(SLID)
ggplot(SLID, aes(education, wages))+geom_point()+labs(title="Scatterplot")
```

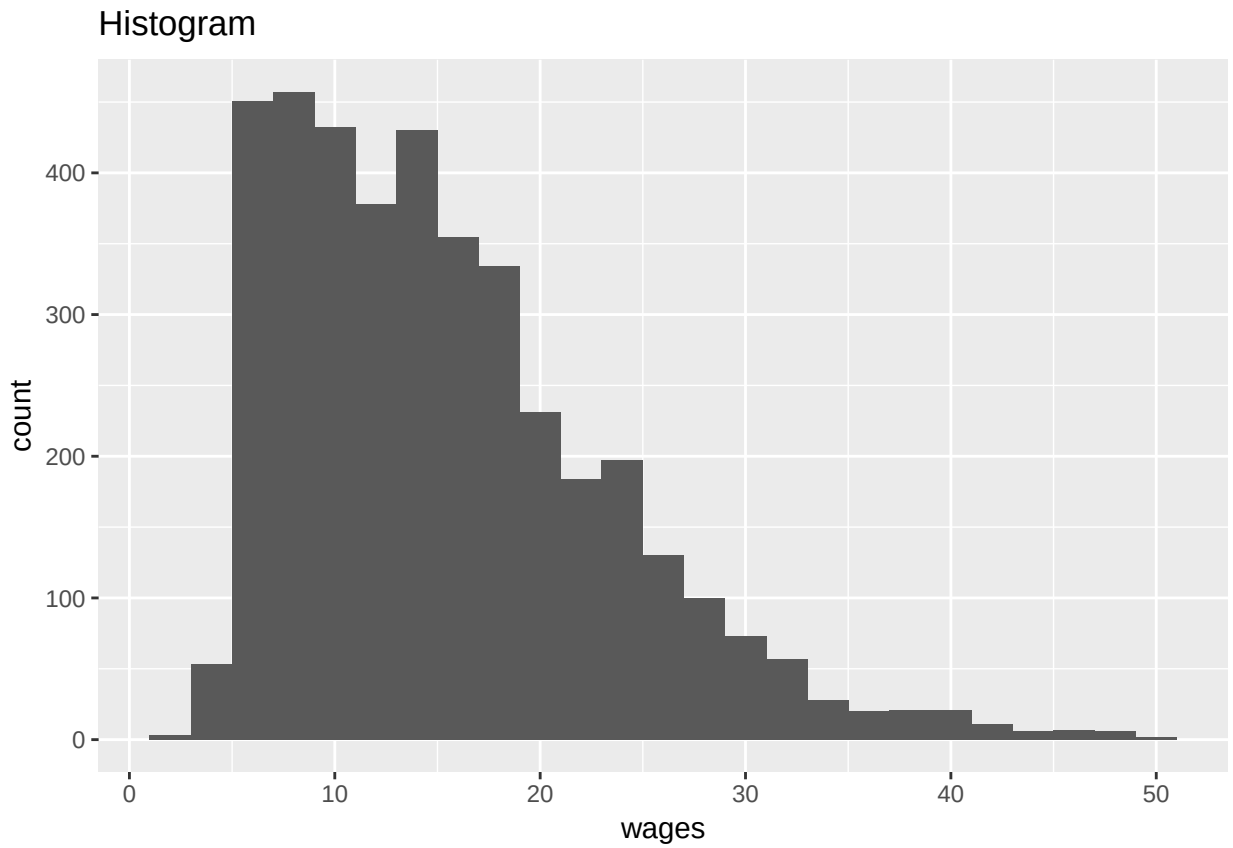



```
ggplot(SLID, aes(education, wages)) + geom_point(aes(color = language)) +
  scale_x_continuous("Education")+
  scale_y_continuous("Wages")+
  theme_bw() + labs(title="Scatterplot") + facet_wrap( ~ language)
```



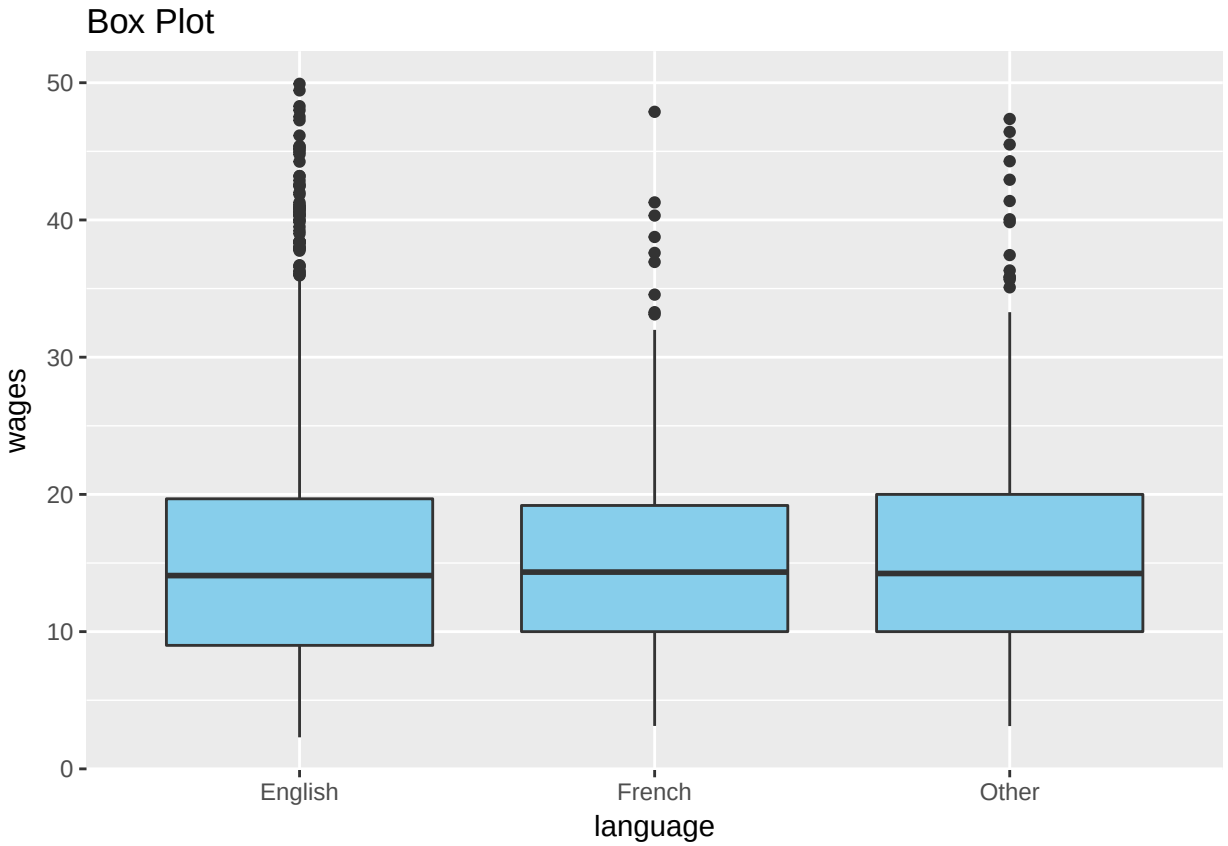
Histogram

```
ggplot(SLID, aes(wages))+geom_histogram(binwidth=2)+labs(title="Histogram")
```



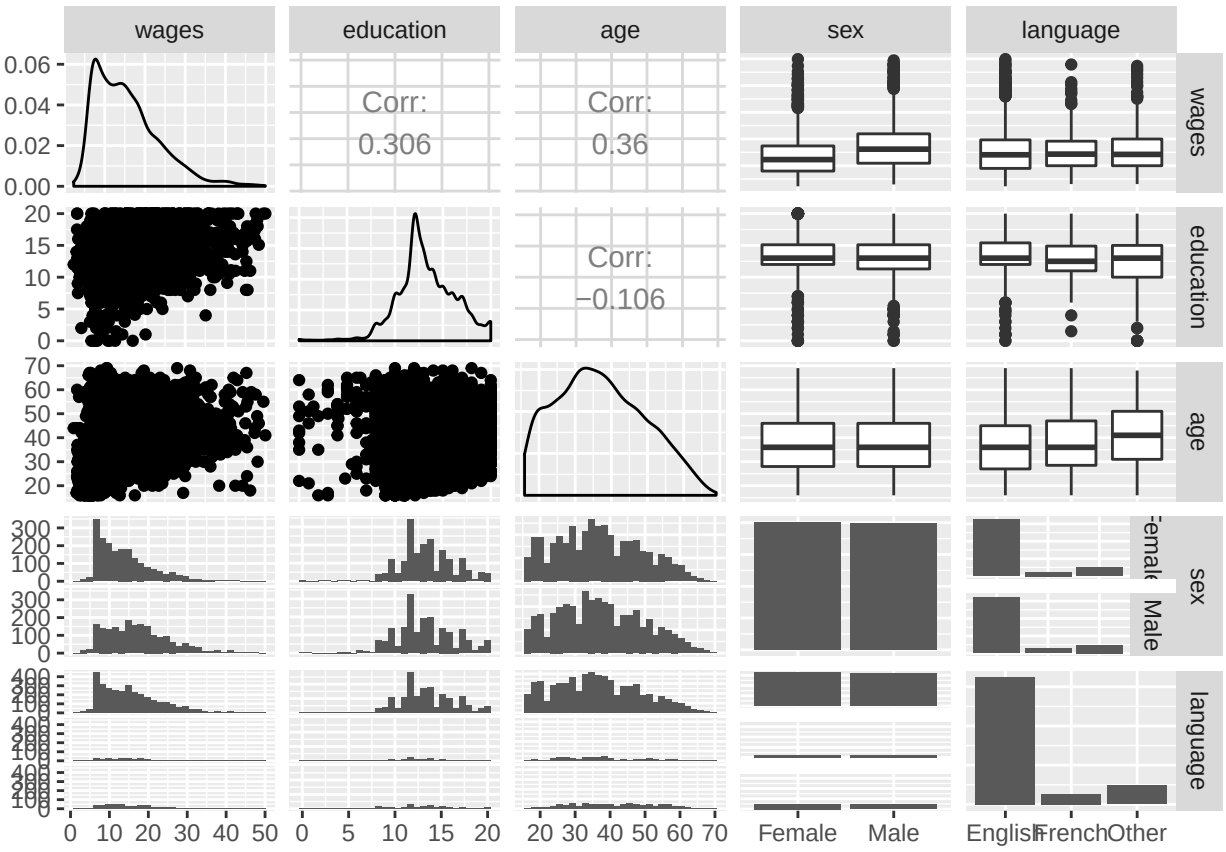
Box-plot

```
ggplot(SLID, aes(language,wages ))+geom_boxplot(fill="skyblue")+labs(title="Box Plot")
```



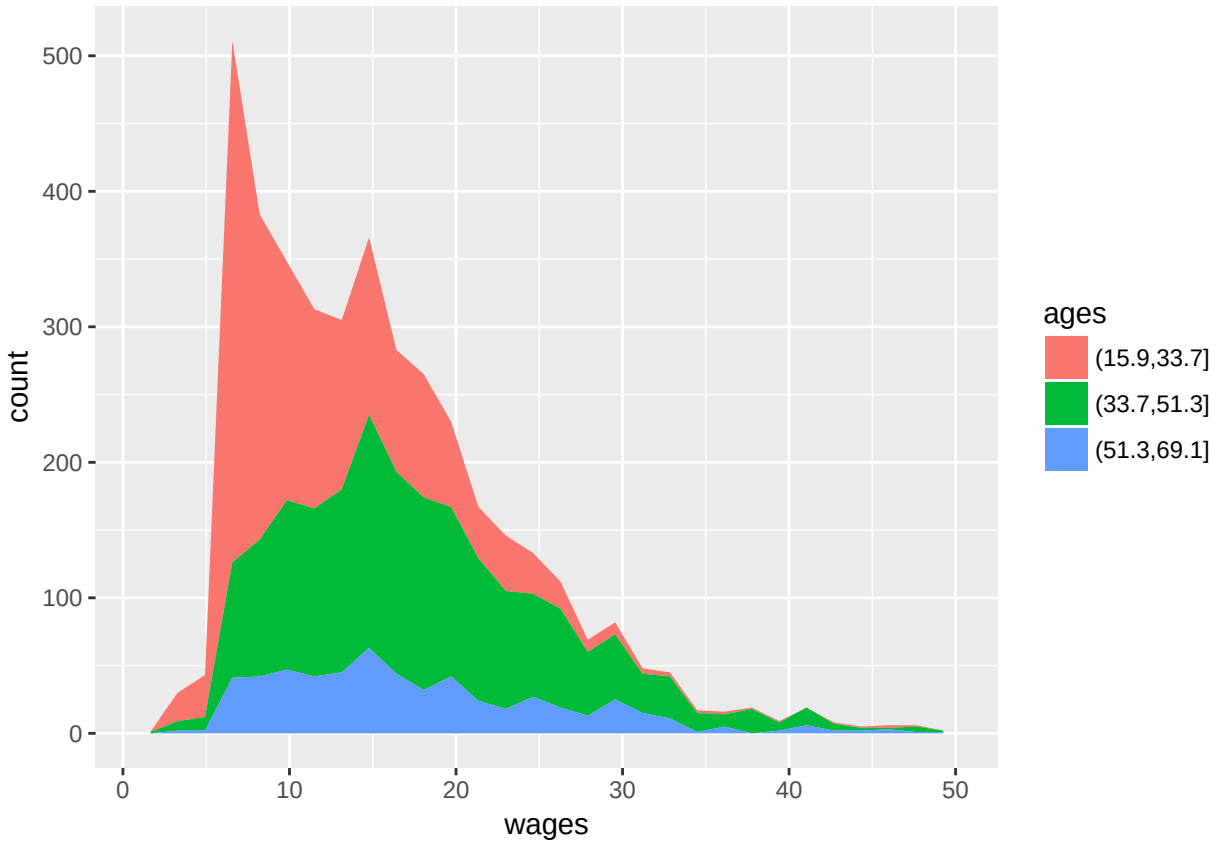
All pairs and different plots

```
library(GGally)
ggpairs(SLID)
```



Area chart

```
ages = cut(SLID$age, breaks=3)
SLID2 = cbind(SLID, ages)
ggplot(SLID, aes(x=wages, fill=ages))+geom_area(stat="bin")
```

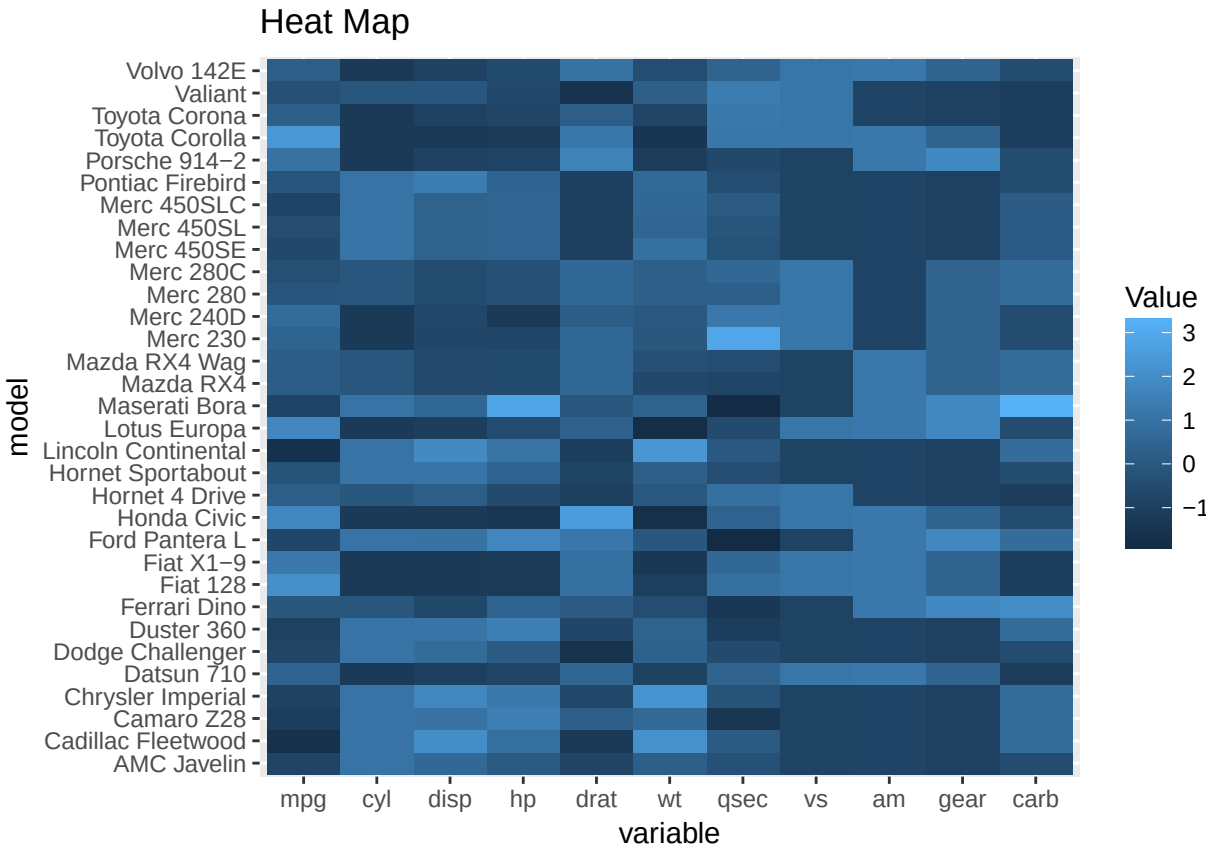


Heat map

```
library(reshape)
head(mtcars)
```

```
##                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
## Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
## Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
## Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
## Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
## Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
## Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

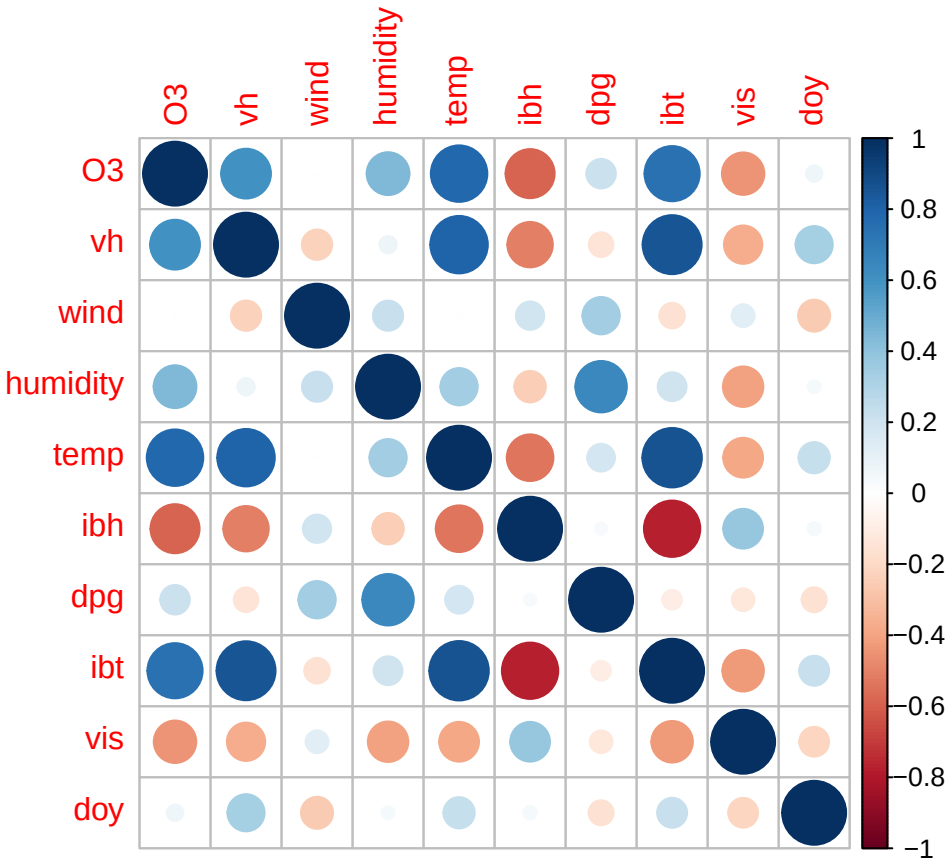
```
carsdf = data.frame(scale(mtcars))
carsdf$model = rownames(mtcars)
cars_melt = melt(carsdf, id.vars="model")

ggplot(cars_melt, aes(x =variable, y = model))+geom_raster(aes(fill=value))+labs(title="Heat Map") + sca
```



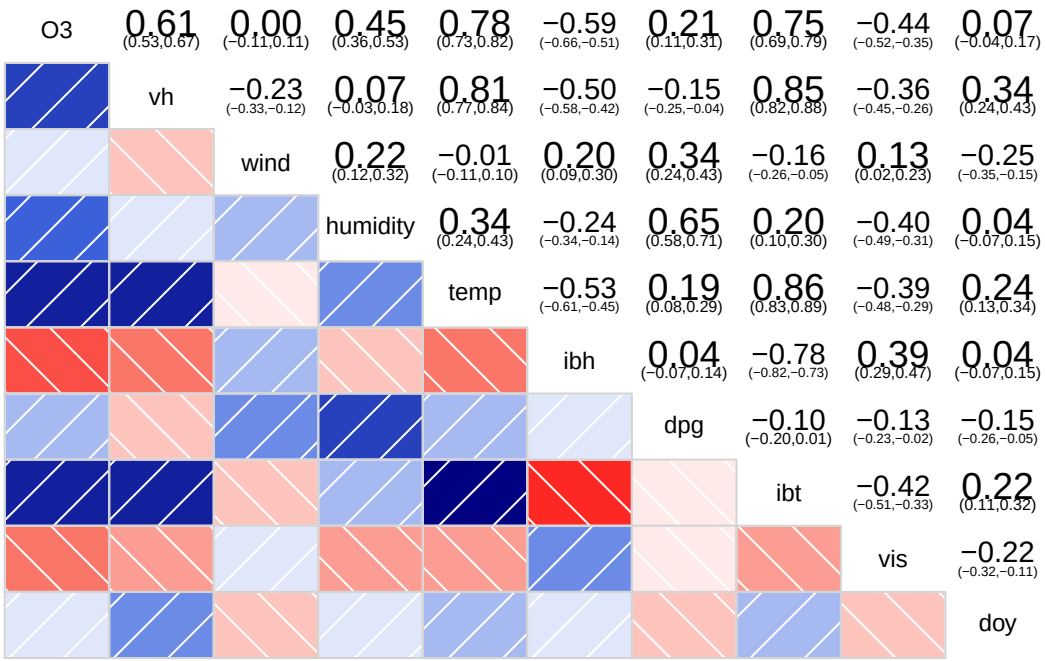
Correlogram

The `ozone` data:

```
library(faraway)
data(ozone)
library(corrplot)
ozonecorr = cor(ozone)
corrplot(ozonecorr)
```




```
library(corrgram)
corrgram(ozone, upper.panel=panel.conf)
```



Further reading/resources

- Videoes on YouTube by the authors of ISL, Chapter 2

R packages to install

```
# packages to install before knitting this R Markdown file
install.packages("knitr")
install.packages("kableExtra")
install.packages("rmarkdown")
install.packages("devtools")
library(devtools) # before installing from github
install_github("yixuan/prettydoc") #nice html-page
install_github("yixuan/xaringan") # nice slides with remark.js
#install.packages("prettydoc") # alternative to github
install.packages("ggplot2")
install.packages("ggpubr")
install.packages("ElemStatLearn")
install.packages("GGally")
install.packages("mvtnorm")
install.packages("MASS")
install.packages("car")
install.packages("faraway")
install.packages("reshape")
install.packages("corrplot")
install.packages("corrgram")
```