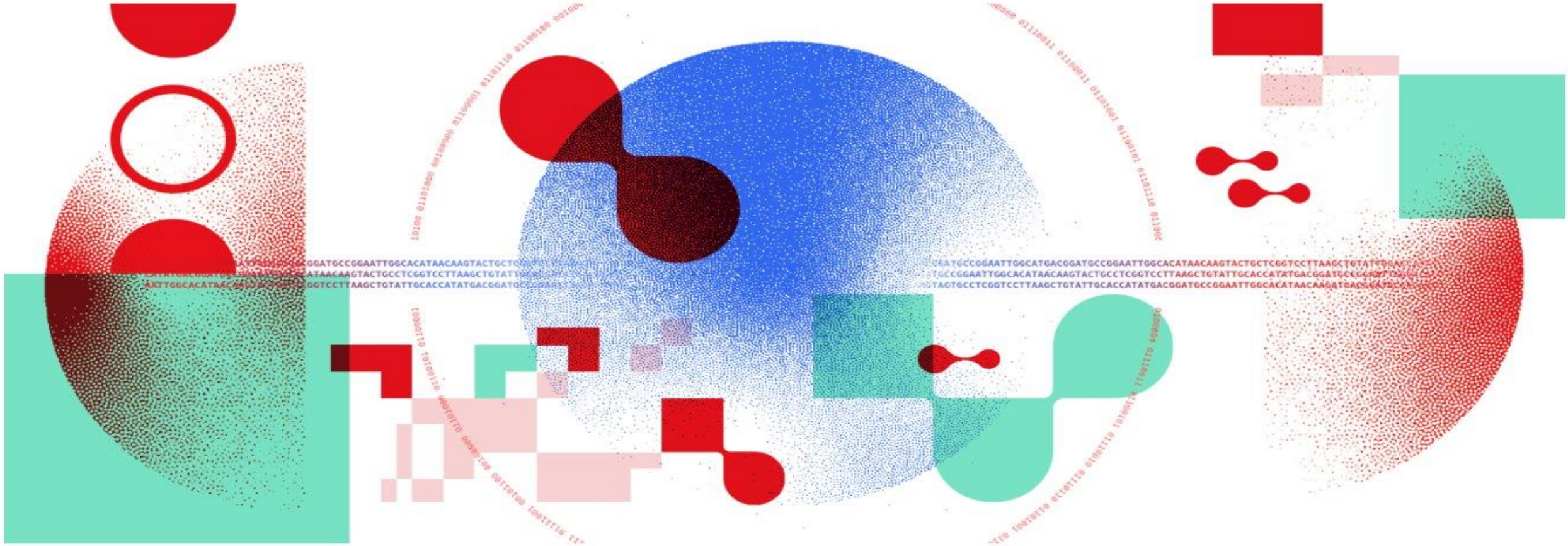

Advanced Statistical Modelling

Lausanne, September 2025

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Caret Day

Plan

- Model Performance
- Sensitivity-Specificity
- ROC curve and Area under the ROC curve (AUC)
- Regularization
- k-fold Cross validation and Leave-one-out method (L1O)
- Signatures

Model Performance-General rules

- We have seen so far that if you compare two models that are nested you can use ANOVA between the two models.
- In order to describe the best model (at least so far), there are measures to describe how good the model is.
- You can use the sum of the residuals, the AIC or BIC, or you could split the original data into a test and training set, assess the parameters on the training set and can therefore use the training set to understand how good the model is. This is often used and there are several measurements that can be retrieved using this method.

AIC

BIC

RSME

MAE

Binomial data- Special case

- Accuracy
- Kappa

Sensitivity vs Specificity

- **Sensitivity** = **true positive rate**, This measures the proportion of individuals with the disease (or value 1 in the dummy category) who are correctly identified as positive by the test.
- **Specificity** = **true negative rate**, is the percentage of persons without the disease (or value 0) who are correctly excluded by the test.

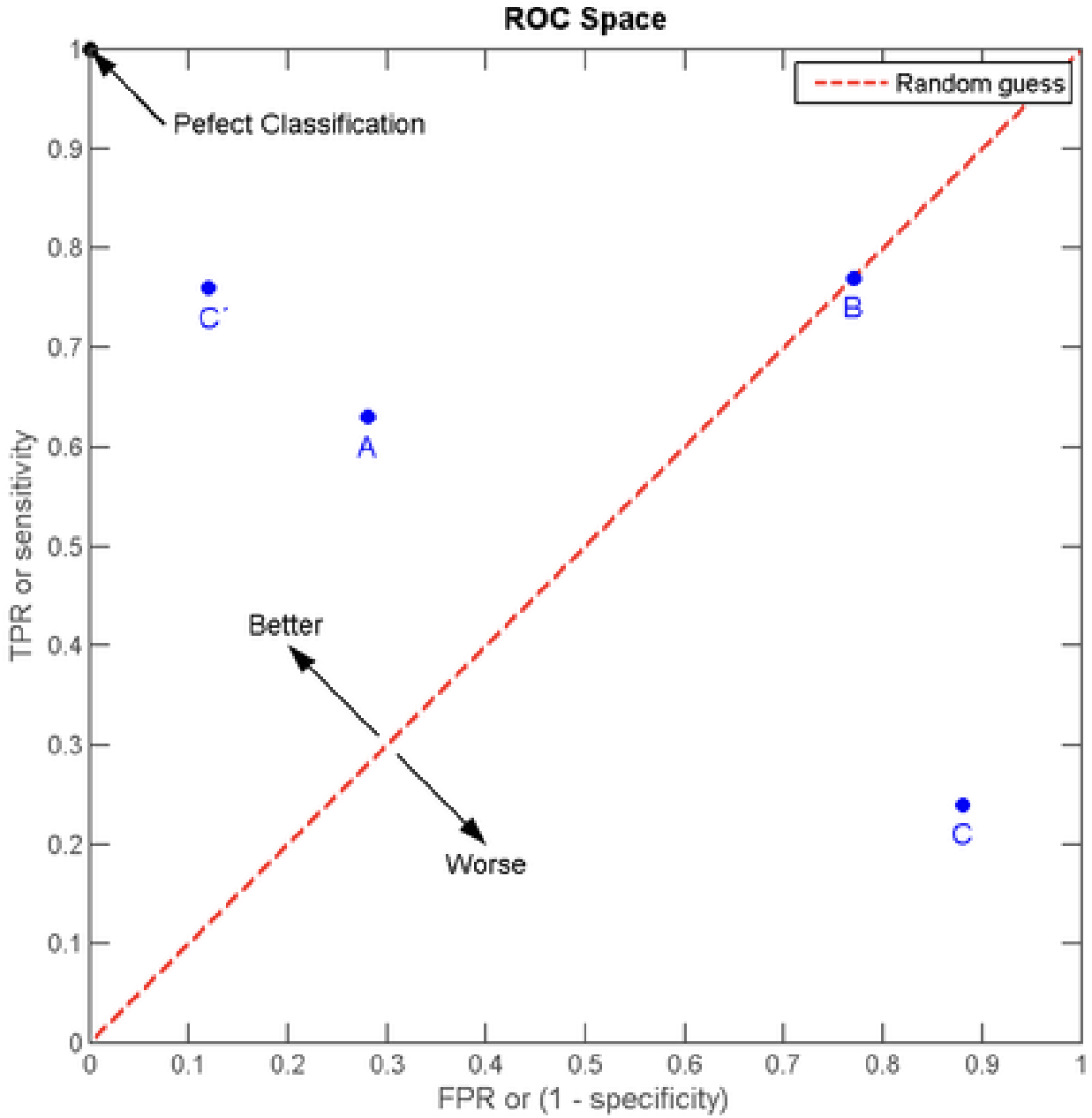
- **High sensitivity**:
- Good at detecting disease, even if it might miss some true negatives (false positives).
- **High specificity:**
- Good at excluding disease, even if it might miss some true positives (false negatives).

- Cancer diagnostic test often have a high **sensitivity** but a lower specificity (because then they get confirmed with a biopsy or secondary test) (specifically for instance with the PSA blood test in prostate cancer)
- Pregnancy test might be more important to have a high specificity because you do not want nonpregnant women to be called pregnant with the pregnancy test even if then you might miss some women that are pregnant, and the test said not pregnant.

ROC curve

- The receiver operating characteristic curve, or ROC curve, is a **graphical plot** that illustrates the performance of a binary classifier model at varying threshold values.
- The ROC curve is the plot of the true positive rate (TPR) against the false positive rate (FPR) at each threshold setting.
- The TPR = sensitivity
- The FPR = 1-specificity (called also probability of false alarm)

ROC



*wikipedia, ROC curve

"I only have my data, how can I make several points for my ROC curve"

- 1. Calculate the probability for all the elements in your test set (predict function in R with type ="response").
- 2. Sort them.
- 3. Now for each value in the response vector you will calculate the number of TP/TN rates and these will be the points in your ROC curve. (Using for example ROCR::prediction and ROCR::performance)
- 4. These values are used to draw the curve.

Example in R using ROCR package

```
> true_labels <- c("P","H","P","H","H")
> predict_proba <- c(0.03,0.1,0.8,0.9,0.95)
> predi <- ROCR::prediction(predict_proba,predict_file)
> perf <- ROCR::performance(predi,x.measure="spec",measure="sens")
> perf@x.values
[[1]]
[1] 1.0000000 0.6666667 0.3333333 0.3333333 0.0000000 0.0000000

> perf@y.values
[[1]]
[1] 0.0 0.0 0.0 0.5 0.5 1.0
```

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```

First we start with the cutoff Infinity. Meaning I have predicted all the samples to be **healthy** : specificity = 1, sensitivity = 0

Then the cutoff will be 0.95 so all my samples will be H except the last one, which is predicted wrongly to be a patient : Specificity = 2/3 healthy are correct, Sensitivity = 0, none of the patient have been identified as patients

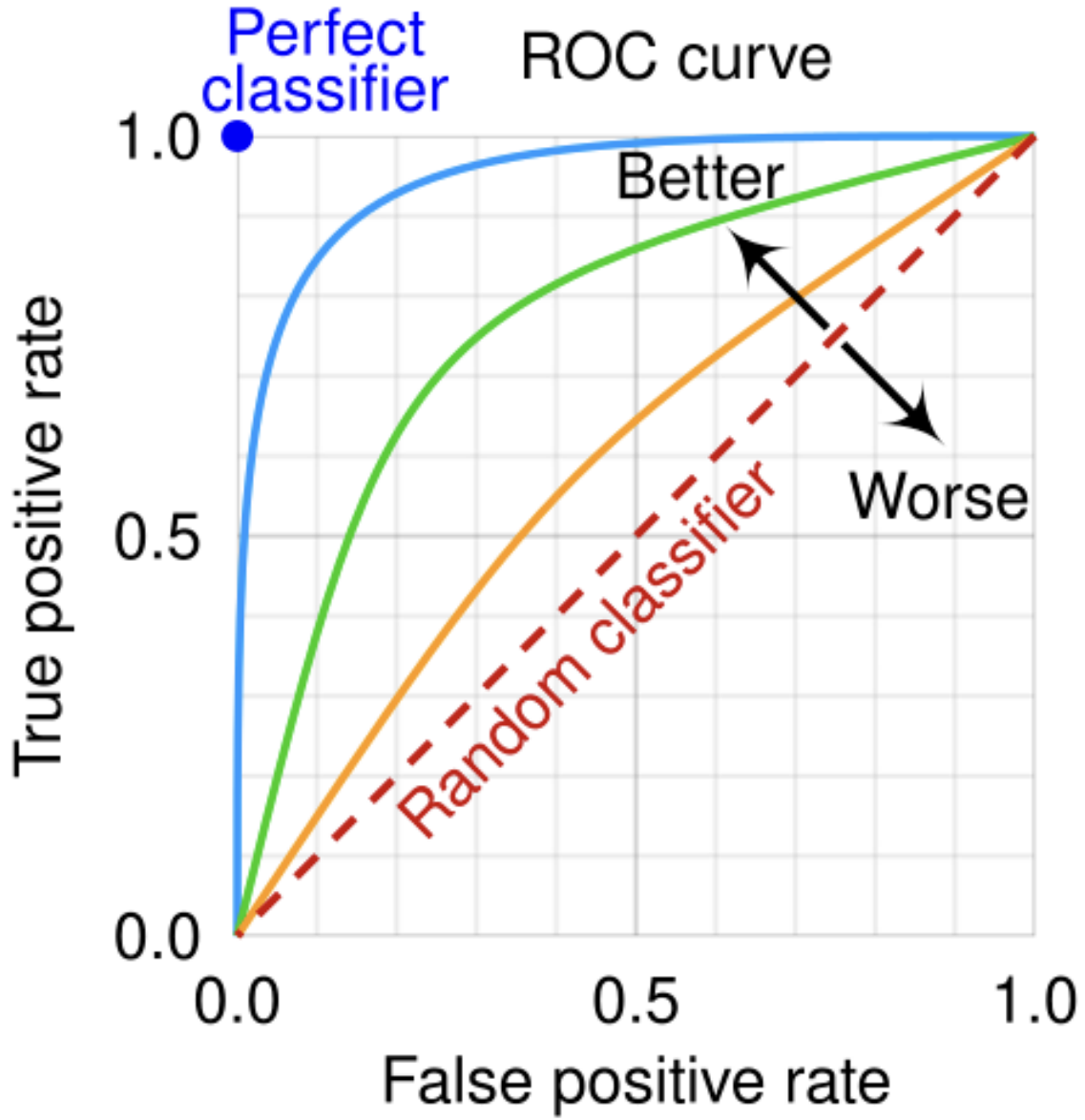
Then cutoff will be 0.9 so all my samples except the last two are considered H, the last two are P : Spec = 1/3 healthy are correct, sensi = 0 none of the P are correct

Then the cutoff will be 0.8, so first two are H last 3 are patients, now my Spec = 1/3 and my sensi = ½

Then cutoff of 0.1, only my first is H all the others are P. The speci= 0, the sensi = ½

Last all the samples are called P and I have a spec= 0,sensi = 1

ROC



*wikipedia, ROC curve

AUC

- Area under the curve or area under the ROC curve.
- A perfect AUC would be of a square 1x1 = 1
- A really random classifier would be giving you a value on the red line, and therefore an AUC of 0.5
- Then, the AUC should always be between 0.5 and 1.

- What happens if your AUC is below 0.5 ? This means you have a higher number of false positives and a lower number of true positives, i.e. the better model would be with inversing all the samples that are called 1 and 0.

Why AUC should not be used, although it often is

- "A method of comparing the areas under receiver operating characteristic curves derived from the same cases." Hanley and Neil 1983 describes how to compare AUC of ROC curves and therefore performance of predictors on same cases.
- However AUC is a summary of the ROC curve with only one value and therefore you miss all the obtained information.
- AUC is also not able to show overfitting or understand the implied measurements.
- Still 1. It is a measure often used in machine learning
- 2. There are many papers trying to convince why it should not be used anymore

Accuracy and Kappa

- Accuracy = (Number of Correct Predictions) / (Total Number of Predictions)
- Does not tell you about if it is better at predicting 1 or 0s and is not telling you either about the balance between the two
- Overall measure of performance

- Kappa = measures the **agreement between predicted and actual class labels**, adjusted for agreement occurring by chance.

$$\kappa = \frac{p_o - p_e}{1 - p_e}$$

Where:

- p_o = observed accuracy (same as regular accuracy).
- p_e = expected accuracy by random chance.

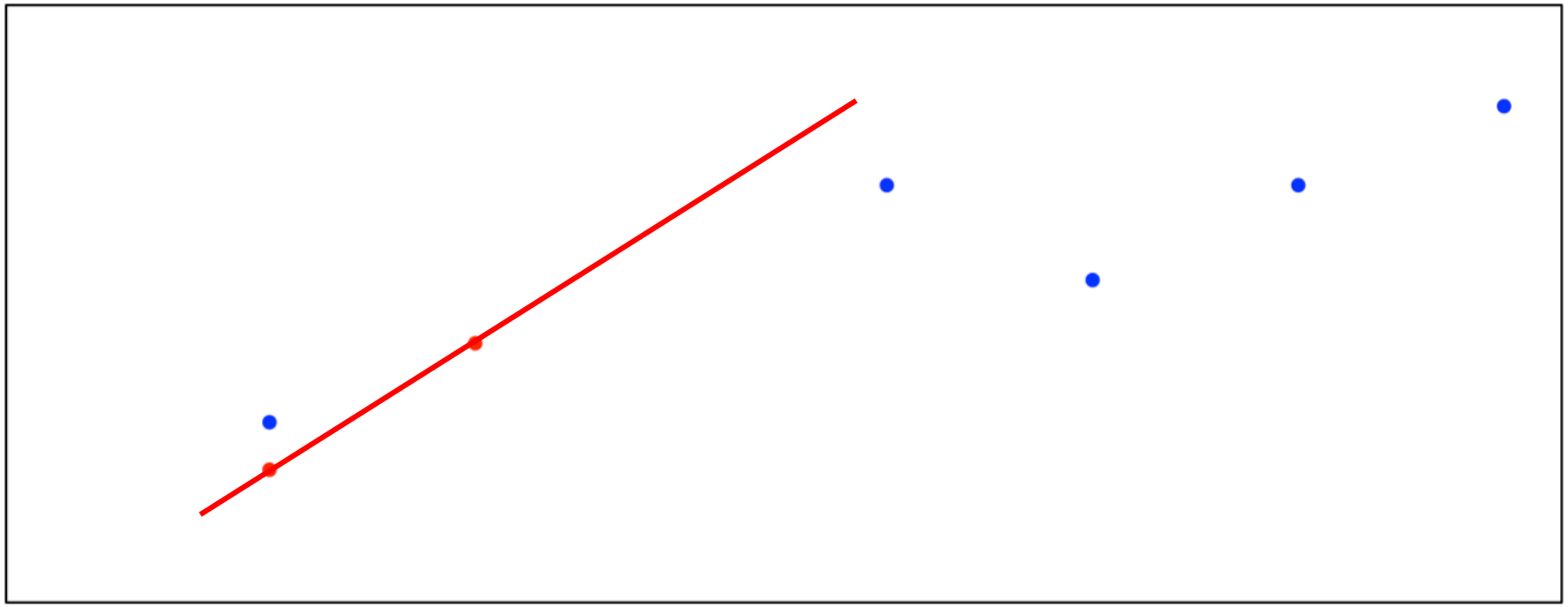
$$p_e = (p_{A1} \cdot p_{P1}) + (p_{A0} \cdot p_{P0})$$

Where:

- p_{A1}: Proportion of actual class 1
- p_{P1}: Proportion of predicted class 1
- p_{A0}: Proportion of actual class 0
- p_{P0}: Proportion of predicted class 0

Regularization

- The goal is to better predict knowing you might not have a good look at the full picture (enough points to predict the real situation).



Regularization

- Regularization are regression that optimize function with a penalty on the coefficients that are used for prediction of the outcome.
- This reduces the variance in the data and reduce overfitting and getting a better balance for the parameters.
- Some regularization will "remove" coefficients that are unnecessary for the regression
- Regularization methods seek to both minimize the sum of squared error of the model on the training data (using ordinary least squares) but also to reduce the complexity of the model

Check out Josh Starmer's channel

- https://www.youtube.com/watch?v=Q81RR3yKn30 (Ridge Regression)
- https://www.youtube.com/watch?v=NGf0voTMlcs (Lasso Regression)
- https://www.youtube.com/watch?v=1dKRdX9bfIo&t=208s (Elastic net Regression)
- https://www.youtube.com/watch?v=fSytzGwwBVw (cross validation)

- https://www.youtube.com/watch?v=iJE2fZcNPlA&t=149s (lecture comparing the 3 first)

3 popular methods

- Lasso Regression (least absolute shrinkage and selection operator): Ordinary least squares is modified to also minimize the absolute sum of the coefficient (called also L1-regularization)
- Ridge Regression: Ordinary least squares is modified to also minimize the squared sum of the coefficient (called also L2-regularization)
- Elastic Net Regression : A combination of both of the above.

- Useful when : you have many parameters that you want to use to predict the model, when you have colinearity, or when you want to be more sure of the prediction you do.

Formulas

$$\sum_{i=1}^{n}(Y_i - \sum_{j=1}^{p} X_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

$$\sum_{i=1}^{n}(y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

$$\hat{\beta} \equiv \underset{\beta}{\operatorname{argmin}}(\|y - X\beta\|^2 + \lambda_2 \|\beta\|^2 + \lambda_1 \|\beta\|_1).$$

What can this help us do

- First of all, the parameter lambda that has been estimated, gives us an information about how much parameters needed tuning and how correlated the predictors were .
- If Lambda is high => lot of correlation => might be wise to do a 2by2 correlation plot to understand which information are correlated
- If Lambda is low => almost like doing a standard regression.

Generate a signature

- After having found a list of N favourite genes that should be able to discriminate your two condition (for example Healthy vs Disease) you can already try to see how they perform in univariate modelling.
- But usually, the idea is to build a signature using part of those N genes.
- We can then put these N genes into our new model and with elastic net regression for example find which genes are not necessary.

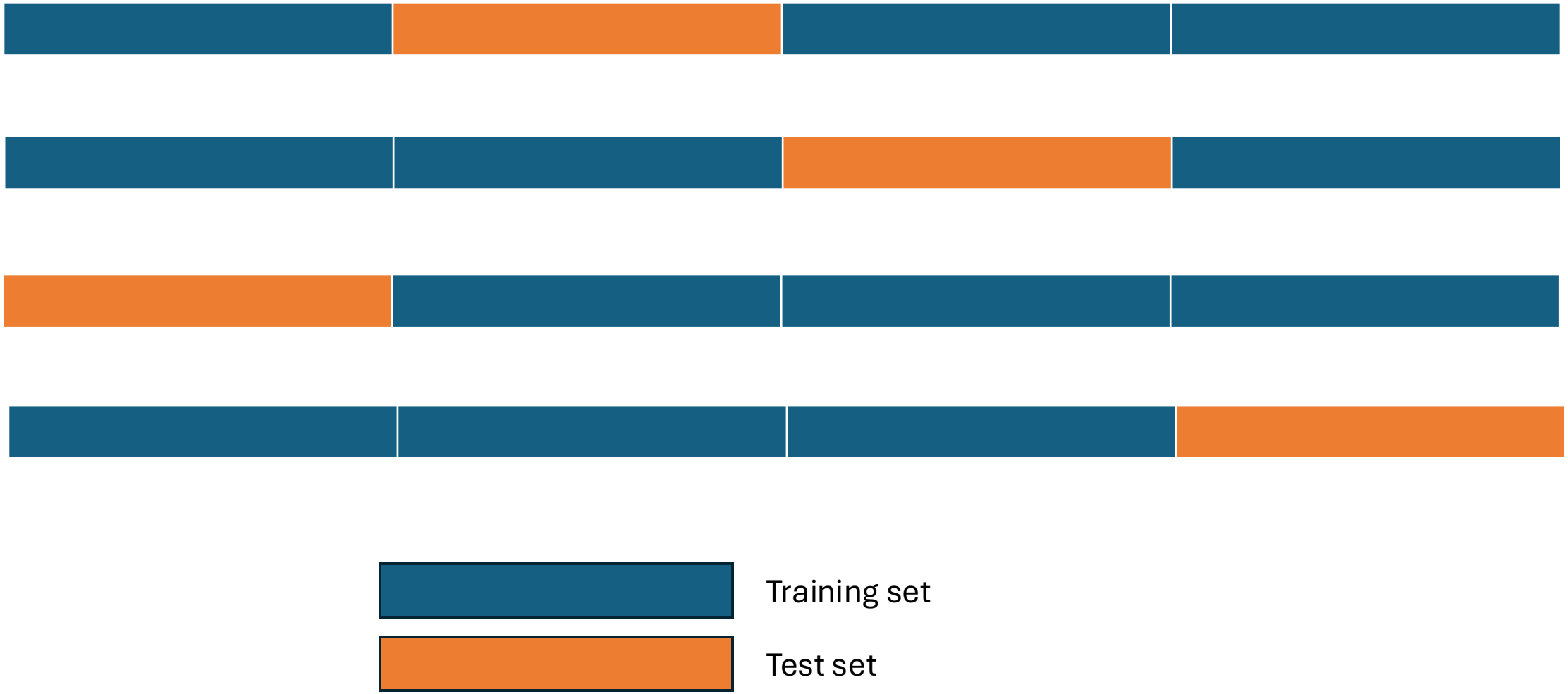
Cross validation

- … or how to have a number on how accurate the model is.
- … or how to know how the model varies according to the points that are included
- … or how to select a model
- … or how to exclude variables
- … or how to show overfitting
- … or how to assess how good the model is

Cross validation explained

- Separates the dataset into a training and a test set
- Train the model (i.e. find the coefficients) on the training set.
- Test the model (i.e. find the outcome) for the test set and see how accurate the model is

K-Fold cross validation with N repetitions



CV repeated in R

```
trC.lm <- trainControl(                  #defines the CV procedure
                 method = "repeatedcv",  #multiple CV
                 number = 5,             #5-fold CV
                 repeats = 10)           #repeats the cross validation 10 times

#fits the linear model with CV defined above
model.lm <- train(bmd ~ age + sex + bmi,
                  data = bmd.data,
                  method = "lm",
                  trControl = trC.lm)
```

CV concretely in the case of (G)LMs

1. It is computing a model based on each of the folds.
2. It then tests the test set with the model and parameters estimated in point 1.
3. It averages the measures of the model through all the folds and this gives an estimation of how good the model is. For LM for instance this would be RSME or R^2 or MAE
4. It then re-estimates the parameters based on the full dataset, which can be obtained using model.lm$finalModel

CV in the case of binomial fits

- The measure in the case of binomial fits is ROC curves, specificity and sensitivity. Either one of those could be of higher importance.

```
trC <- trainControl(
            method = "cv",     #just 1 CV
            number = 10,       #10-fold CV
            classProbs = TRUE,
            summaryFunction = twoClassSummary,
            savePred =TRUE)  #to be used in the confusion matrix

model.LR <- train(fract ~ age + sex + bmi + bmd ,
                data = bmd.data, method = "glm",
                family="binomial",
                trControl = trC,
                metric = "ROC")



# Model Summary
model.LR
```

The resultsmodel.LR$results

- With model.LR$results we obtain the average ROC, average sensitivity and average specificity measured on the test set of each folds as well as the standard deviation of them.

Parameters

- `PreProcess can be used`
- Sensitivity
- specificity

KNN-method

- Method of K-nearest-neighbours.
- For example k=3, it would look for the 3 closest neighbours in the data and do an averaging for regression or a most-common result for categorical values.
- The choice of k can be taken from a grid of possibilities with the parameter : tuneGrid= expand.grid(k = c(3, 5, 7, 9, 11)).

Fruit classification

- Suppose you want to classify a new fruit based on weight and color:
- Your training data has labeled fruits: apples, oranges, bananas
- For a new fruit, KNN finds the 3 (k=3) closest fruits according to the model done with weight and color in the training data
- If 2 are apples and 1 is an orange, the new fruit is classified as an **apple**

KNN is very dependent on the number K and very dependent on the data. To check the stability of the result use CV

Random Forest