

Model Evaluation

Machine Learning for Behavioral Data

March 21, 2022

Today's Topic

Week	Lecture/Lab
1	Introduction
2	Data Exploration
3	Regression
4	Classification
5	Model Evaluation
6	Time Series Prediction
7	Time Series Prediction
8	Time Series Prediction

Complete pipeline for one use case:

- Data exploration
- Prediction
- Model evaluation

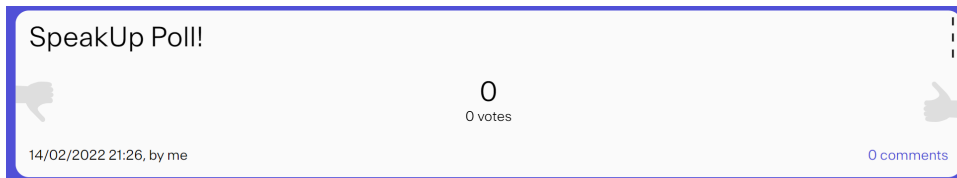
Getting ready for today's lecture...

- **If not done yet:** clone the repository containing the Jupyter notebook and data for today's lecture into your Noto workspace
- SpeakUp room for today's lecture:

<https://go.epfl.ch/mlbd-lecture>

Short quiz about the past...

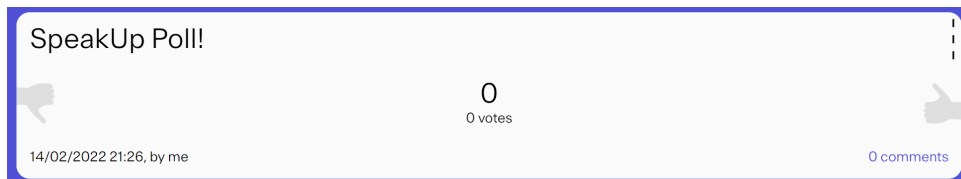
[Classification] Which of the following is an example of an ensemble method?



- a) Decision Tree
- b) k-Nearest Neighbor
- c) Logistic Regression
- d) Random Forest

Short quiz about the past...

[Classification] We are going to predict the species of an Iris Flower. The dependent variable (species) contains three possible values: Setosa, Versicolor, and Virginica. Which classification methods are appropriate for this task?

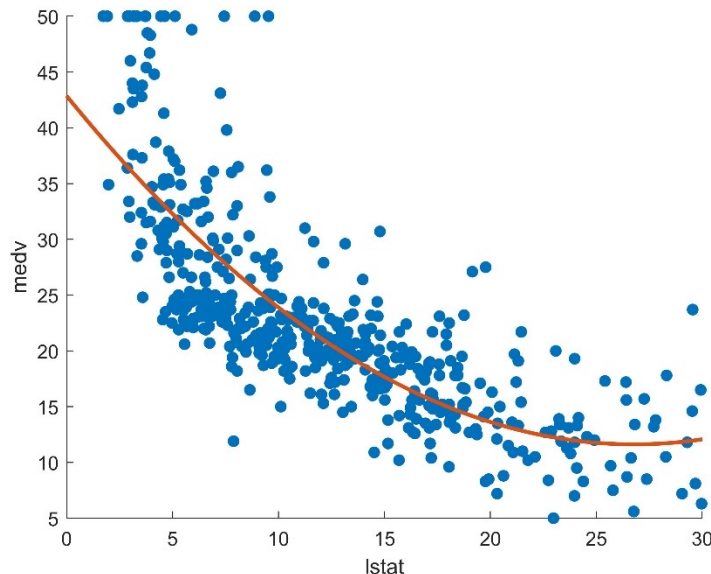


- a) Decision Tree
- b) k-Nearest Neighbor
- c) Logistic Regression
- d) Random Forest

Today

- **Model Assessment and Selection**
 - Reporting of Results
-

How good is my model?



$$medv = 42.86 - 2.33 \cdot lstat + 0.04 \cdot lstat^2$$

$$R^2 = 0.64$$

SpeakUp Chat!



0
0 votes



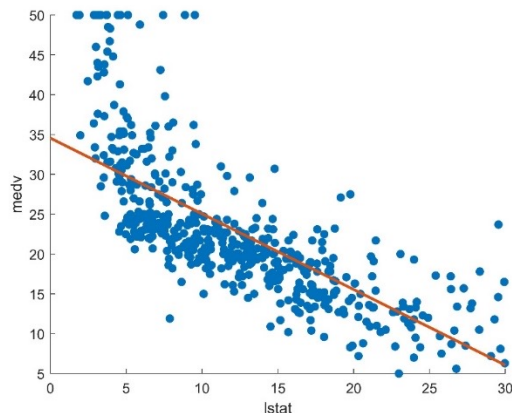
14/02/2022 21:25, by me

0 comments

lstat: Percentage of lower status of the population

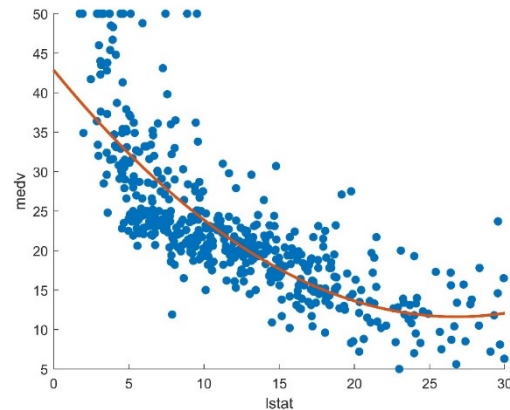
medv: Median value of owner-occupied homes in \$1000s

Which model is better?



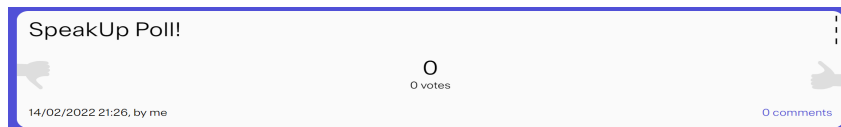
$$medv = 34.55 - 0.95 \cdot lstat$$

$$R^2 = 0.54$$



$$medv = 42.86 - 2.33 \cdot lstat + 0.04 \cdot lstat^2$$

$$R^2 = 0.64$$



- a) The left model
- b) The right model
- c) I need more information

Model Evaluation

- **Model assessment**: having chosen a final model, estimating its prediction error on new data (*generalization*).
-

Model Evaluation

- **Model assessment:** having chosen a final model, estimating its prediction error on new data (*generalization*).
 - **Model selection:** estimating the performance of different models in order to choose the best one.
-

Theory: Notation

- We are given a sample data set:

$$T = \{(y_n, \mathbf{x}_n)\} \text{ with } n = 1, \dots, N$$

- The sample data set T has been drawn from an **(unknown)** underlying data model D with range $X \times Y$:

$$(y_n, \mathbf{x}_n) \text{ i.i.d. } \sim D$$

- We have learnt a model f for predicting y based on \mathbf{x} . How good is f ?
-

Theory: Expected Loss

$$Err_D(f) = E_D[L(y, f(\mathbf{x}))]$$

where y and \mathbf{x} are randomly drawn from D , i.e. $Err_D(f)$ is the *expected* error of f over all samples chosen according to D . $Err_D(f)$ is denoted as *expected/true risk/loss*.

Theory: Expected Loss

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where y and \mathbf{x} are randomly drawn from D , i.e. $Err_D(f)$ is the *expected* error of f over all samples chosen according to D . $Err_D(f)$ is denoted as *expected/true risk/loss*.

- We cannot compute $Err_D(f)$, since we don't know D .
 - We are, however, given a sample data set T , drawn from D . We can use T to approximate the expected loss.
-

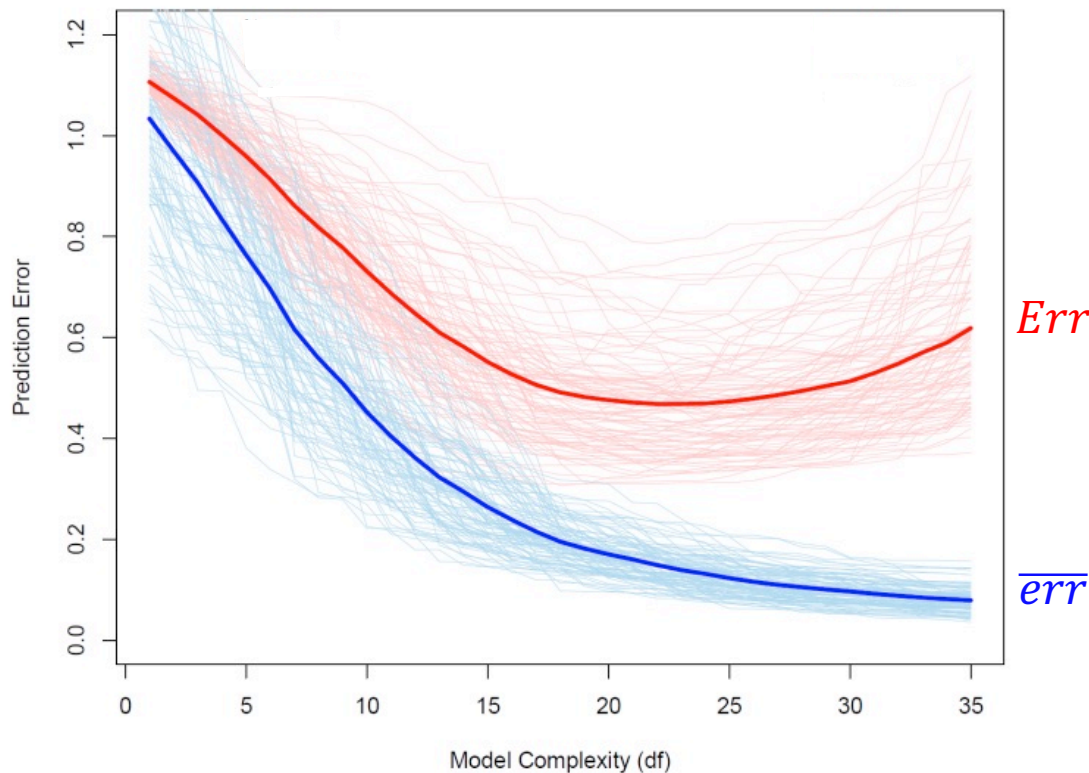
Theory: Training Error

- First idea: we compute the error of f on T to *empirically* approximate $Err_D(f)$:

$$\overline{err}(f) = \frac{1}{|T|} \sum_{(x_n, y_n) \in T} L(y_n, f(x_n))$$

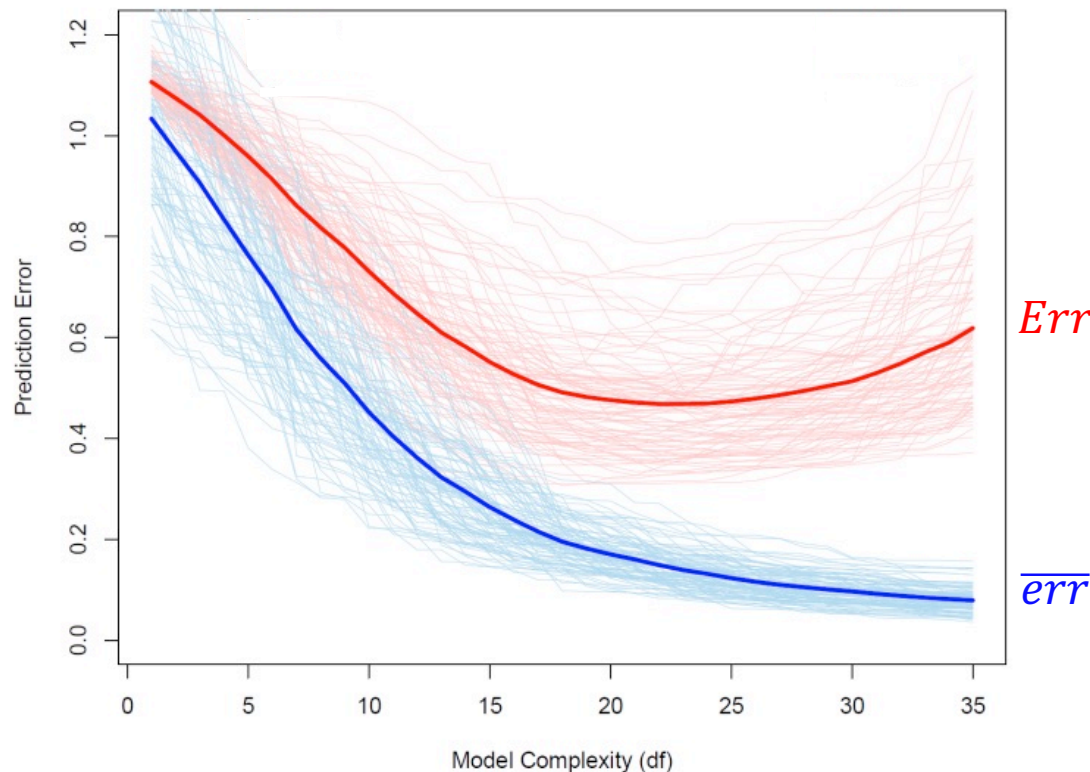
- We call $\overline{err}(f)$ the *empirical error* (or simply the *training error*).
-

Training error underestimates expected loss



- Using synthetic data, we can compute the expected loss (we **know** D).

Training error underestimates expected loss



- Using synthetic data, we can compute the expected loss (we **know** D).
- The training error underestimates the expected loss



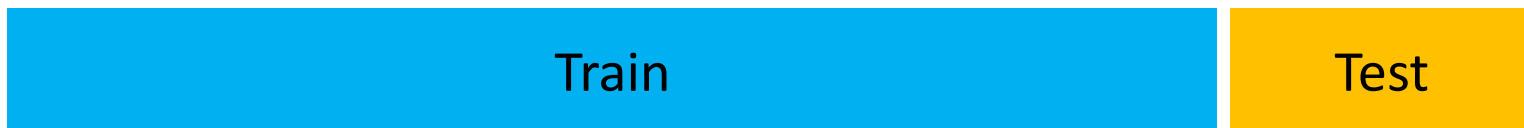
We need a better solution to estimate Err_D

Model Assessment & Selection

- ① **Train, Validate, Test**
 - ② Resampling Methods
 - ③ Information Criteria
-

Fixed assignment

- We randomly split the data into a training data set and a test data set (e.g., 80/20 split or 70/30 split)



- *Training set*: used for fitting the model
 - *Test set*: assessment of the generalization error of the model
-

Test Error

- We randomly split the data set T into a training data set and a test data set (e.g., 80/20 split or 70/30 split)

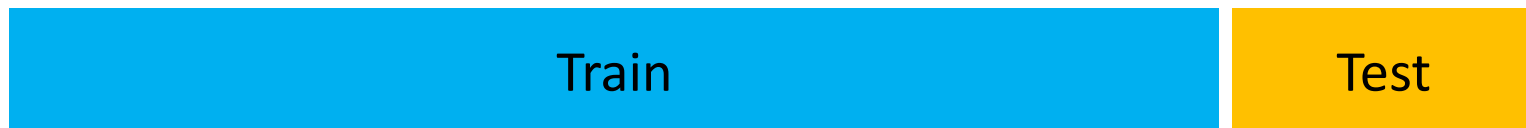
Train

Test

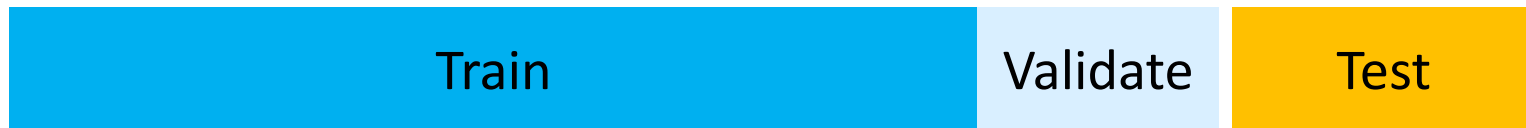
$$Err_{test}(f_{train}) = \frac{1}{|T_{test}|} \sum_{(x_n, y_n) \in T_{test}} L(y_n, f_{train}(x_n))$$

Fixed assignment: Selection & Generalization

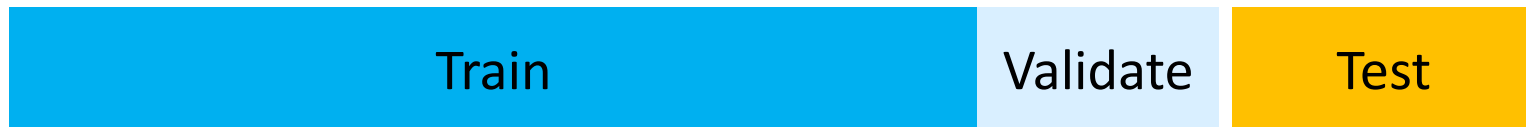
- We randomly split the data set T into a training data set and a test data set (e.g., 80/20 split or 70/30 split)



- We further (randomly) split the training data set T_{train} and reserve a part of it for validation (e.g., 80/20 split)



Fixed assignment: Selection & Generalization



- *Training set*: used for fitting the models
 - *Validation set*: used to estimate the prediction error for model selection (e.g., hyperparameter tuning)
 - *Test set*: assessment of the generalization error of the chosen model
-

Inefficient use of data



- Not very efficient use of data (requires a large amount of data)
 - How large? Depends on
 - Signal to noise ratio of data set
 - Complexity of the models we want to fit
-

Assessment & Selection

- ① Train, Validate, Test
 - ② **Resampling Methods**
 - Cross Validation
 - Bootstrapping
 - ③ Information Criteria
-

K-Fold Cross-Validation

- Randomly divide data into K parts (folds)
- For $k = 1, \dots, K$
 - Fit the model to the other $K - 1$ folds $\{1, \dots, K\} \setminus \{k\}$
 - Compute the prediction error on k
- Combine the K estimates of prediction error

$K = 5$



k = 1	Test	Train	Train	Train	Train
k = 2	Train	Test	Train	Train	Train
k = 3	Train	Train	Test	Train	Train
k = 4	Train	Train	Train	Test	Train
k = 5	Train	Train	Train	Train	Test

Combining the K estimates of prediction error

$K = 5$



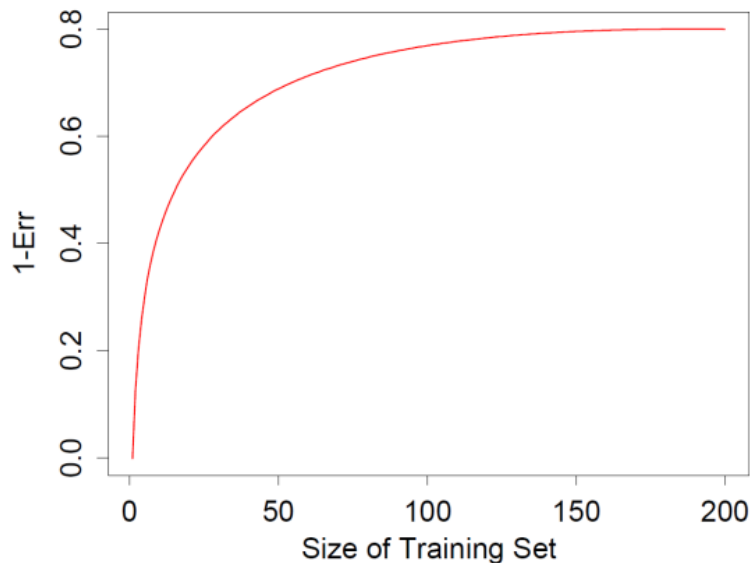
k = 1	Test	Train	Train	Train	Train
k = 2	Train	Test	Train	Train	Train
k = 3	Train	Train	Test	Train	Train
k = 4	Train	Train	Train	Test	Train
k = 5	Train	Train	Train	Train	Test

$$PE^{CV} = \frac{1}{K} \sum_{k \leq K} PE_k = \sum_{i=1}^N L(y_i, f^{-\kappa(i)}(x_i))$$

Leave-one-out cross validation

- $K = N$, i.e. each fold just contains one sample
 - For a sample i , we train f on all samples but i and then use f to predict on i
 - Can have high variance (the N training sets are very similar to each other)
 - High computational burden (f needs to be fit N times)
 - Avoids issues with fold selection
-

How do we choose K?



- We don't know the learning curve of our model
 - In practice: 5-fold and 10-fold cross validation are recommended as a good compromise
-

Variants of cross validation

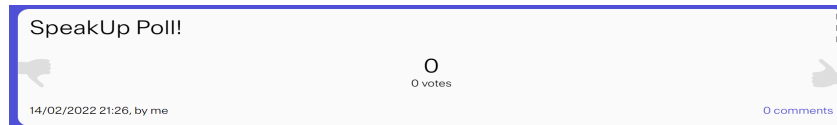
- Flat
 - Each sample has equal chance of being placed into each fold
 - Stratified
 - Fold selection is biased such that some variable is equally represented in each fold
 - This can be the variable we are trying to predict (y)
 - This can be a variable that is thought to be an important context
-

Stratification

- Other levels of stratification are possible (e.g., school, learning environment, demographic information)
 - Consideration:
 - Where will the model be used (e.g., what is the potential application)?
 - Make sure you stratify at this level
 - Can also be combined (e.g., we can stratify by predicted variable y and by user)
 - Stratification can also be used in the fixed assignment (train – validate – test) setting
-

Example: Classification Problem

- Given: classification problem, synthetic data set with
 - **binary** class label y (balanced)
 - 5000 features (*independent* of class labels y)
- What is the expected loss of any classifier f on this data set?



- a) 10%
- b) 30%
- c) 50%
- d) 70%
- e) 90%

Example: Suggested Procedure

- 1) Select the 100 features that have the highest correlation with the class labels y
- 2) Use a 1-nearest neighbor classifier based on just these 100 selected features
- 3) Use cross validation to estimate the prediction error of the classifier

➡ Over 50 simulations of this procedure: $PE^{CV} = 0.03$

Be careful!

- Multistep modeling procedure
 - Cross-validation must be applied to the **entire sequence** of modeling steps. In particular, **samples must be “left out” before any selection or filtering steps** are applied.
 - Exception: **unsupervised** cleaning or screening steps can be done before samples are “left out”.
 - This of course holds also for the train-validate-test case!
-

Your Turn – Model Assessment

- In your student notebook, we provide examples on Train-Test Split and Cross Validation model evaluation.
 - Your task:
 - Run the Train-Test Split and the Cross Validation model evaluations
 - What is the difference in accuracy/AUC between the two methods?
Where does this difference come from?
-

Assessment & Selection

- ① Train, Validate, Test
 - ② **Resampling Methods**
 - Cross Validation
 - **Bootstrapping**
 - ③ Information Criteria
-

Bootstrapping

- General tool for assessing statistical accuracy
 - Basic idea:
 - Given: training data set $\mathbf{Z} = \{z_1, \dots, z_N\}$ with $z_i = (\mathbf{x}_i, y_i)$, where N is the number of samples
 - Randomly draw N pairs (\mathbf{x}_i, y_i) with replacement from the training data set
 - Repeat B times (e.g., $B = 100$) $\rightarrow B$ bootstrap data sets
 - Fit model to each bootstrap data set, observe behavior across bootstrap data sets
-

Bootstrapping

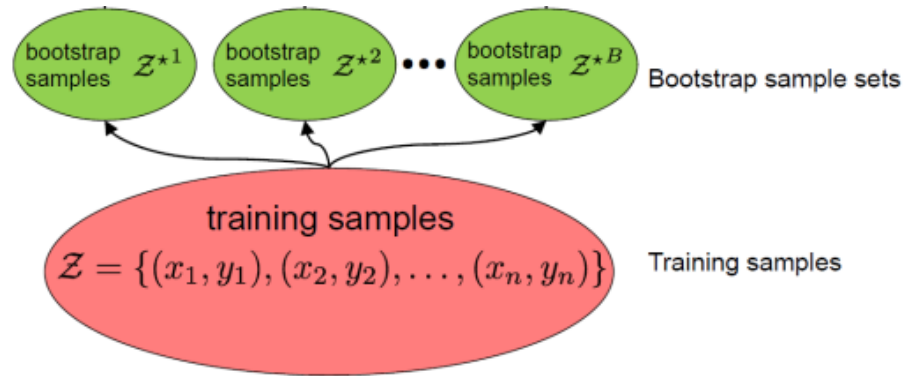
- We are interested in $S(Z)$
- $S(Z)$ can be any quantity computed from the data Z , e.g., the prediction at some input point
- We want to compute an aspect of the distribution of $S(Z)$ (e.g., the variance)

training samples

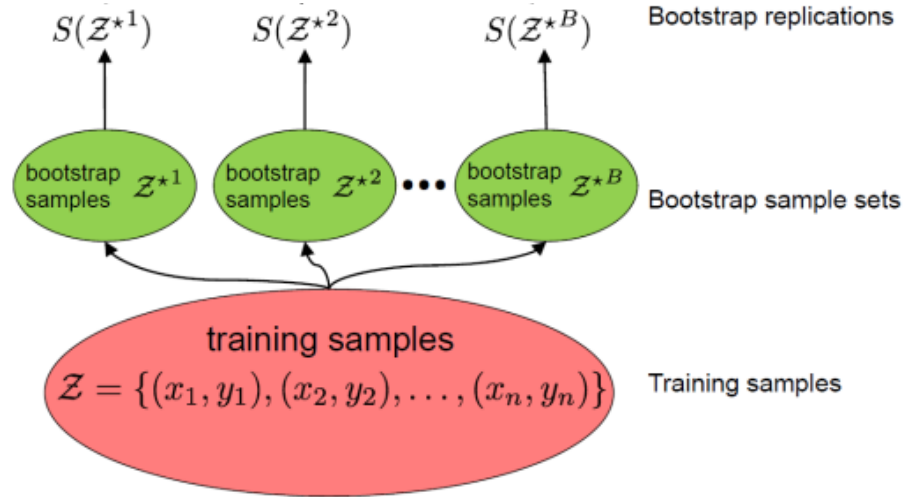
$$Z = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

Training samples

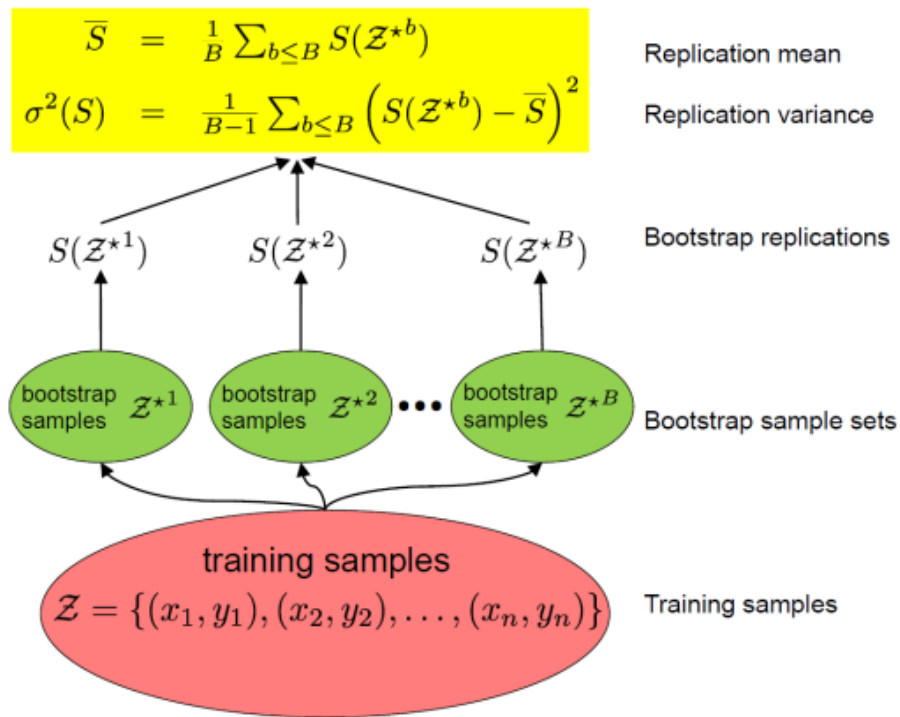
Bootstrapping



Bootstrapping



Bootstrapping



Bootstrapping for prediction

- Idea: leave-one-out bootstrap

$$\widehat{Err}^{(1)} = \frac{1}{N} \sum_{i=1}^N \frac{1}{|C^{-i}|} \sum_{b \in C^{-i}} L(y_i, f^{*b}(\mathbf{x}_i))$$

where C^{-i} denotes the set of indices of bootstrap samples b , that do **not** contain observation i

.632 bootstrap error

- It can be shown that the average number of distinct samples in each bootstrap sample b is about $0.632 \cdot N$
- $\widehat{Err}^{(1)}$ will therefore tend to overestimate the true loss
- Solution:

$$\widehat{Err}^{(.632)} = .368 \cdot \overline{err} + .632 \cdot \widehat{Err}^{(1)}$$

Assessment & Selection

- ① Train, Validate, Test
 - ② Resampling Methods
 - ③ **Information Criteria**
 - AIC
 - BIC
-

Information Criteria

- The training error is an overly optimistic estimate of the *expected loss*
 - Information criteria try to estimate the *optimism* in the training error and correct for it
-

Akaike Information Criterion (AIC)

$$AIC = -\frac{2}{N} \cdot \loglik + 2 \cdot \frac{d}{N}$$

- d is the number of parameters of our model f
 - \loglik is the log-likelihood (logarithm of the likelihood) of the sample data T given our model f
 - N is the number of samples in the data set, i.e. $|T| = N$
-

Bayesian Information Criterion (BIC)

$$BIC = -2 \cdot \loglik + \log(N) \cdot d$$

- d is the number of parameters of our model f
 - \loglik is the log-likelihood (logarithm of the likelihood) of the sample data T given our model f
 - N is the number of samples in the data set, i.e. $|T| = N$
 - BIC penalizes complex models more heavily than AIC
-

Information Criteria - Considerations

- Applicable for models where the fitting is done under a maximum likelihood setting
 - *Effective* number of parameters:
 - Choosing the best fitting model with d features, can result into more than d parameters being fit (e.g., regularization)
 - Determining the *effective* number of parameters can be difficult for more complex models (e.g., trees)
-

What method should we choose?

- ① Train, Validate, Test
 - ② Resampling Methods
 - Cross Validation
 - Bootstrapping
 - ③ Information Criteria
 - AIC
 - BIC
-

What method should we choose?

Depends on the purpose of the model:

- Interpretation: information criteria are useful for unsupervised cases or when the model is built for interpretation purposes (e.g., which features of the regression model explain the data better?)
 - Prediction:
 - All presented methods (train-test, cross validation, bootstrap) are reasonable choices
 - We can combine them freely to do model selection and assessment
 - In practice: while bootstrap provides accurate estimates of test error, it also requires a high amount of extra work
-

Example Combinations



Your Turn – Model Selection & Assessment

- In your student notebook, we provide three examples on how to tune to hyperparameters of the model and then evaluate the prediction error of that model in terms of accuracy or AUC
 - Your task:
 - Find the incorrect example and tell us why they are incorrect
 - Fix the incorrect example. How does the prediction error change?
-

Your Turn - Feedback

- In your student notebook, we provide five examples on how to tune to hyperparameters of the model and then evaluate the prediction error of that model in terms of accuracy or AUC
- Your task:
 - Find the two incorrect examples and tell us why they are incorrect
 - Fix at least one of these examples. How does the prediction error change?

Upload your Jupyter Notebook here to get feedback:

<https://go.epfl.ch/mlbd-activities>

Today

- Model Selection and Assessment
 - **Reporting of Results**
-

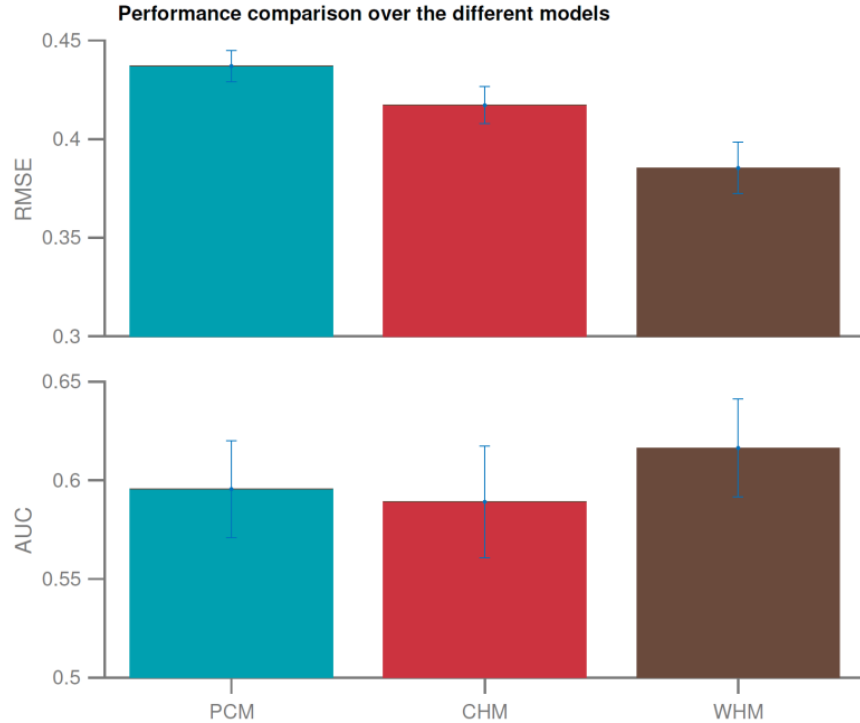
Back to the question: is my model any good?

- A friend tells you that he has found a great model for early prediction of drop out in online courses
 - She gives you the following information:
 - The data set stems from N students taking course c
 - 30% of the students dropped the course
 - She has evaluated her model using cross validation
 - The accuracy of the model is 0.8 and the AUC is 0.83
-

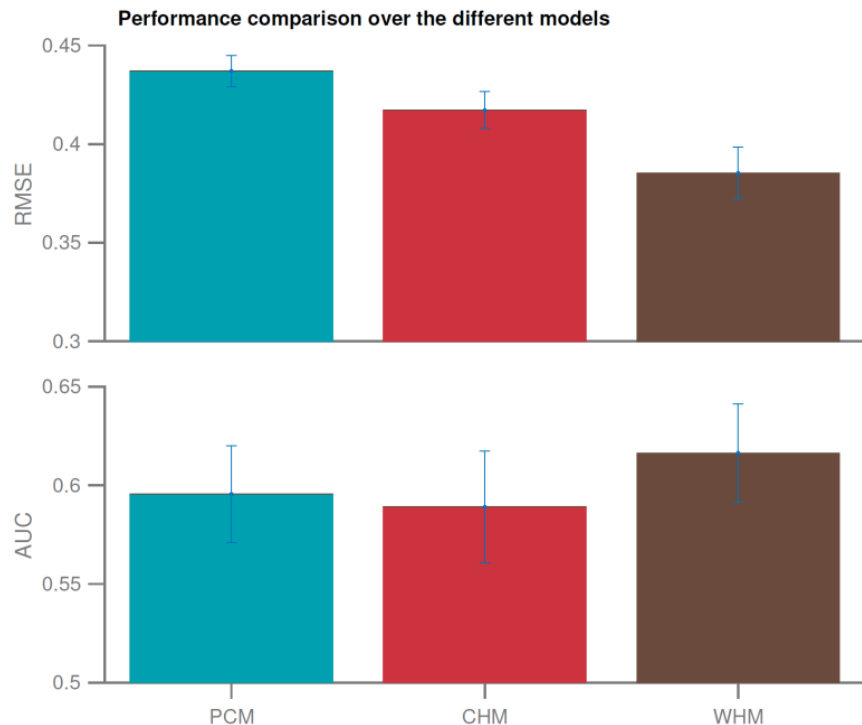
Provide comparisons!

- Reporting performance metrics for a model f on a data set T is not enough: achievable performance (what is good?) depends on the data set!
 - We need to provide comparisons to **baseline** models:
 - **Minimum** baseline: compare to a random model
 - Additional comparisons, depending on the goal:
 - Suggestion of a new type of model structure for a problem: need to compare to previously suggested structures
 - Suggestion of new features for a problem: need to compare performance between a model using and not using the new features
-

Quantification of Uncertainty



Quantification of Uncertainty



- We usually report the *mean* prediction error over all samples
- We should quantify the uncertainty of the performance metric!
- Uncertainty can be computed across samples where applicable (or across folds)
- Error bars can denote
 - Standard deviation
 - Standard error ($\sqrt{\sigma^2/N}$)

Today

- Model Assessment and Evaluation
 - Reporting of Results
-

Summary: Pipeline

Design/choose an appropriate learning algorithm and features



- Problem (e.g., classification or regression)
- Data set (e.g., size, type)
- Task (e.g., dropout prediction)

Summary: Pipeline

Design/choose an appropriate learning algorithm and features



Select evaluation method



- Data set (e.g., size and type)
- Learning algorithm (e.g., model complexity)
- Goal (e.g., interpretation or prediction)
- Potential application (e.g., generalization to new users -> stratification)

Summary: Pipeline

Design/choose an appropriate learning algorithm and features



Select evaluation method

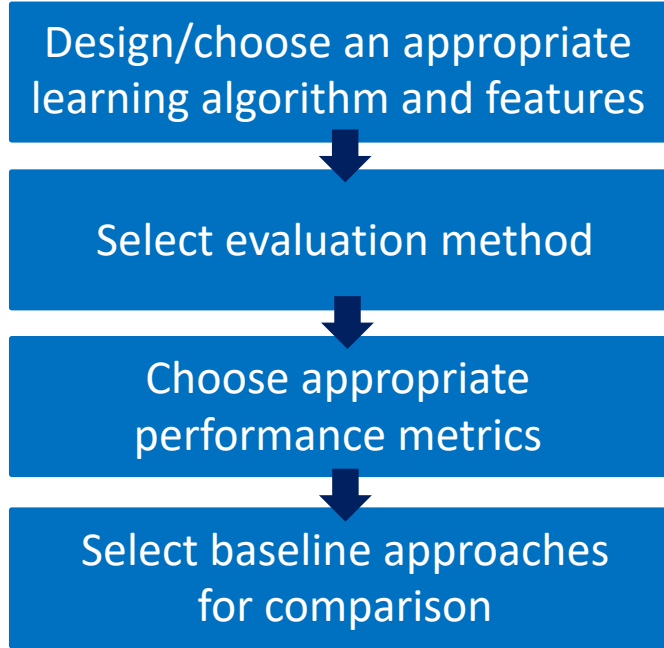


Choose appropriate performance metrics



- Problem (e.g., classification or regression)
- Learning algorithm (e.g., model type)
- Potential application (i.e., what is important?)

Summary: Pipeline



} What do I want to show/prove, i.e. what is my claim (e.g., suggestion of new neural network architecture, suggestion of new features for a specific problem)?

Summary: Pipeline

Design/choose an appropriate learning algorithm and features



Select evaluation method



Choose appropriate performance metrics



Select baseline approaches for comparison



Report your results providing error bars

Summary: Pipeline

Design/choose an appropriate learning algorithm and features



Select evaluation method



Choose appropriate performance metrics



Select baseline approaches for comparison



Report your results providing error bars

There are many ways to solve a given task (e.g., predicting student performance). It is important that:

- You provide a clean and complete evaluation of your solution
- You are able to justify your decisions for each step

If you want additional practice...

- You can solve tasks from last year's homework
 - independently
 - during the tutorial sessions on Wednesday morning, the TAs will be happy to help and answer questions
- For this lecture: [Homework 3 - 2021](#)
- We are happy to provide feedback on your solution:

Upload your Jupyter Notebook here:

<https://go.epfl.ch/mlbd-activities>
