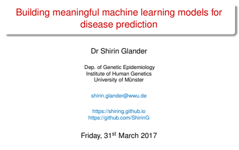
Webinar for ISDS R Group

2017-03-28



Building meaningful machine learning models for disease prediction

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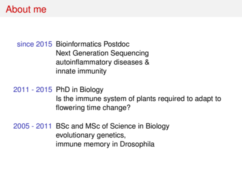
Friday, 31st March 2017

- Welcome everybody!
- Thank you very much for the invitation and the opportunity to present this talk
- I will go over my work on using machine learning models in disease prediction
- I want to specifically give a hands-on demonstration of how you can build meaningful models yourselves using R
- I will demonstrate how to evaluate model performance and
- how to optimize models to address different disease-related questions

About me



About me

since 2015	Bioinformatics Postdoc Next Generation Sequencing autoinflammatory diseases & innate immunity
2011 - 2015	PhD in Biology Is the immune system of plants required to adapt to flowering time change?
2005 - 2011	BSc and MSc of Science in Biology evolutionary genetics, immune memory in Drosophila

- Before I start, I want to quickly introduce myself:
- I am a bioinformatics postdoc
- working with next generation sequencing data,
- like RNA-seq for transcriptomics,
- whole genome sequencing for variant analysis,
- ATAC- or Chip-seq for chromatin and epigenetic information.
- My own research focuses on questions relating to autoinflammatory diseases
- and innate immune mechanisms

- I earned my PhD in biology from the University of Münster in 2015
- working with RNA-seq data to determine how plant defense has co-evolved with and potentially shaped different life-history strategies

- Before that, during my BSc and MSc I worked on questions about evolutionary genetics and immune memory in Drosophila

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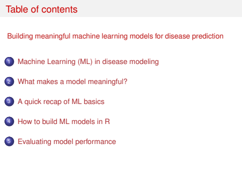

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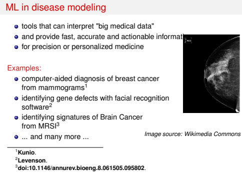
Building meaningful machine learning models for disease prediction

1. Machine Learning (ML) in disease modeling
2. What makes a model meaningful?
3. A quick recap of ML basics
4. How to build ML models in R
5. Evaluating model performance

- Now, let's start with the topic about which you're here:
- Machine learning is a powerful approach for developing sophisticated, automatic, and objective models for the analysis of complex biomedical data
- Machine learning promises to help physicians make near-perfect diagnoses, ...
- ... choose the best medications for their patients, ...
- ... predict readmissions, ...
- ... identify patients at high-risk for poor outcomes, ...
- ... and in general improve patients' health while minimizing costs.

- I titled my talk: "Building meaningful machine learning models for disease prediction"
- with the emphasis on **meaningful**
- So, first, I want to introduce to you what it is I mean exactly with **meaningful models**
- Then, I will give you a few examples of how machine learning is currently being used in disease modeling and clinical data science
- Before I delve into the nitty-gritty of modeling, I will quickly recap the most important concepts of ML
- And finally, I will show how to build ML models in R
- and how to evaluate the performance of such models



ML in disease modeling

- tools that can interpret "big medical data"
- and provide fast, accurate and actionable informat
- for precision or personalized medicine

Examples:

- computer-aided diagnosis of breast cancer from mammograms[1]
- identifying gene defects with facial recognition software[2]
- identifying signatures of Brain Cancer from MRSI[3]
- ... and many more ...

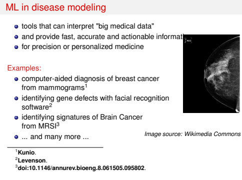
Image source: Wikimedia Commons

[1] **Kunio**.
[2] **Levenson**.
[3] **doi:10.1146/annurev.bioeng.8.061505.095802**.

- there is not a place in medicine where AI doesn’t have potential applications:
- more data is being collected that needs to be interpretated
- increasingly data driven diagnosis, e.g. in radiology
- image recognition of e.g. tumors or pneumonia in medical images
- similar to training ML models to recognize images of cats (classification in images)
- ML allows incorporation of data from heterogenous inputs:
- clinical, genomics, drugs, electronic health records, etc.
- = personalised medicine

- A key aspect of precision medicine is the development of informatics tools
- that can analyze and interpret ’big data’ sets
- in an automated and adaptive fashion
- while providing accurate and actionable clinical information
- ML based models can improve detection, diagnosis, and therapeutic monitoring of disease

- you can find things with ML that you wouldn’t be able to find otherwise
- many models today perform better than humans!
- a patient with a rare difficult condition can be matched to similar cases from the past
- faster diagnosis, better treatment



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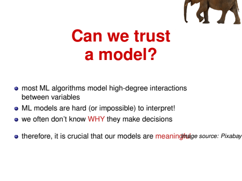
- identifying breast cancer, lung cancer, osteoporosis, brain tumors, etc. from medical images
- predicting response of different cancer types to different treatments
- Computer-Aided Diagnosis (CAD) has become one of the major research subjects in medical imaging and diagnostic radiology
- With CAD, radiologists use the computer output as a ’second opinion’ and make the final decisions
- In vivo magnetic resonance spectroscopy imaging (MRSI) allows noninvasive characterization
- and quantification of molecular markers of potentially high clinical utility
- for improving detection, identification, and treatment for a variety of diseases, most notably brain cancers

- facial analysis technology aids diagnoses of genetic disorders
- researchers at the University of Oxford in the United Kingdom
- Face2Gene uses machine learning
- helps geneticists narrow down possible disorders that often involve dysmorphic facial features

- doctors are still important!
- computer does the tasks that we humans are not good at, like interpreting complex images
- we have more data than humans can manage to make sense of (e.g. genomics data)
- the clinicians will be freed up to think about best treatment options and talk more with the patients
- good models are built on strong knowledge of the question and the biology behind it
- features need to be evaluated in context



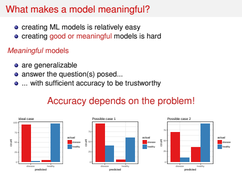
Can we trust a model?

- most ML algorithms model high-degree interactions between variables
- ML models are hard (or impossible) to interpret!
- we often don't know WHY they make decisions
- therefore, it is crucial that our models are meaningful

Image source: Pixabay

- the elephant in the room
- inherent problem with ML models: they are hard (or impossible) to interpret
- machine learning algorithms tend to create nonlinear,
- non-monotonic,
- non-polynomial,
- and even non-continuous functions
- that approximate the relationship between independent and dependent variables in a data set
- most ML algorithms model high-degree interactions between variables (meaning the effect of combining many?i.e., mo than two or three?variables together)

- When working with data you should be asking yourselves some very hard questions:
- do I understand my data?
- Do I understand the model and answers my machine learning algorithm is giving me?
- And do I trust these answers?
- Unfortunately, the complexity that bestows the extraordinary predictive abilities on machine learning algorithms also makes the answers the algorithms produce hard to understand,
- and maybe even hard to trust.
- almost by definition one cannot really understand a good model
- difficulties in interpretation still present a barrier for the widespread, practical use of ML
- trusting models and results is a general requirement for good (data) science
- we want to understand them as well as possible



What makes a model meaningful?

- creating ML models is relatively easy
- creating good or meaningful models is hard

Meaningful models

- are generalizable
- answer the question(s) posed...
- ... with sufficient accuracy to be trustworthy

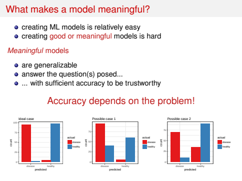
Accuracy depends on the problem!

- With a little bit of practice, anybody can build machine learning models
- what is hard though, is to build 'good' or 'meaningful' models
- I want to begin with an introduction to the main question of my talk:
- what makes a model *good* or *meaningful*?

1. it needs to be generalizable, i.e. it needs to perform well on unseen data
2. It answers a **specific** question or addresses a specific problem,
   e.g. does a mammogram image show a healthy breast or is there a tumor?
   Or does an ECG show a normal heart rhythm or arrhythmia?
3. And it produces a correct outcome (e.g. a diagnosis) often enough that we trust it!

- If we build models, we therefore need to evaluate its accuracy
- before we can decide whether it is trustworthy enough to implement in real-life,
- like in a hospital where it could e.g. assist doctors in making decisions on treatment

- But what exactly is *high accuracy* can not be defined with a one-size-fits-all approach:
- it depends on the problem we want to model.
- a model needs to perform well in the real world, not in the lab (i.e. on training data)
- just because a model performs well in the lab, doesn't mean it will also perform well in deployment
- the context might change: distribution, missing data, noise, class size, etc.



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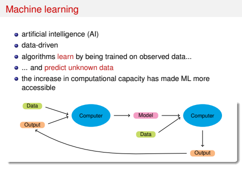
Let me illustrate what I mean with the following examples:

- Ideal case: Of course, we all want to achieve ideal modeling results where overall prediction accuracy is very high. With a model like that, we can be very confident that a healthy person is indeed healthy and a sick person is not.
- But in reality, we often achieve prediction accuracies that are much less nice.
- Scenarios 1 and 2: Le’s consider two possible scenarios:
- in scenario 1, we can be very confident that a person who got classified as "healthy" is indeed healthy, while a person who has been diagnosed as diseased might as well be healthy based on these prediction accuracies
- in case 2, it is the other way around.
- We now need to make a decision which scenario is better and in which direction we want to optimize our model: do we rather want to refer a few healthy people for further checking because the model predicted them as diseased? Or do we rather want to be as certain as possible that a predicted disease is actually true and accept that we might miss a few disease cases?

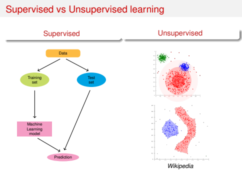


Machine learning

- artificial intelligence (AI)
- data-driven
- algorithms learn by being trained on observed data...
- ... and predict unknown data
- the increase in computational capacity has made ML more accessible

ML concepts are not new, but the increase in computational capacity has made them more accessible
Machine learning is the subfield of computer science that, according to Arthur Samuel in 1959, gives "computers the ability to learn without being explicitly programmed."[1] Evolved from the study of pattern recognition and computational learning theory in artificial intelligence,[2] machine learning explores the study and construction of algorithms that can learn from and make predictions on data[3] ? such algorithms overcome following strictly static program instructions by making data driven predictions or decisions,[4]:2 through building a model from sample inputs. Machine learning is employed in a range of computing tasks where designing and programming explicit algorithms with good performance is difficult or unfeasible; example applications include email filtering, detection of network intruders or malicious insiders working towards a data breach,[5] optical character recognition (OCR),[6] learning to rank and computer vision.
Machine learning is closely related to (and often overlaps with) computational statistics, which also focuses on prediction-making through the use of computers. It has strong ties to mathematical optimization, which delivers methods, theory and application domains to the field. Machine learning is sometimes conflated with data mining,[7] where the latter subfield focuses more on exploratory data analysis and is known as unsupervised learning.[4]:vii[8] Machine learning can also be unsupervised[9] and be used to learn and establish baseline behavioral profiles for various entities[10] and then used to find meaningful anomalies.

Within the field of data analytics, machine learning is a method used to devise complex models and algorithms that lend themselves to prediction; in commercial use, this is known as predictive analytics. These analytical models allow researchers, data scientists, engineers, and analysts to "produce reliable, repeatable decisions and results" and uncover "hidden insights" through learning from historical relationships and trends in the data.[11]



Supervised vs Unsupervised learning

Supervised

Unsupervised

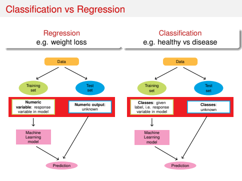
Wikipedia

- Unsupervised:
- no input!
- matrix decomposition methods, e.g. nonnegative matrix factorization
- pattern recognition
- clusters data into different groups
- able to recover biomarkers of disease and toxicity

- Supervised
- classification labels are given
- e.g. support vector machine

- Semi-supervised:
- a little bit of input, like how many classes to find

Here, I will focus on supervised learning!



Classification vs Regression

Regression
e.g. weight loss

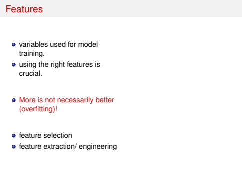
Classification
e.g. healthy vs disease

Data
Training set
Test set
Numeric variable: response variable in model
Numeric output: unknown
Machine Learning model
Prediction
Data
Training set
Test set
Classes: given label, i.e. response variable in model
Classes: unknown
Machine Learning model
Prediction

- Supervised learning!
- Your learning algorithm seeks a function from inputs to the respective targets.
- If the targets are expressed in some classes, it is called classification problem.
- Alternatively, if the target space is continuous, it is called regression problem.

- Functions created by linear regression algorithms are probably the most interpretable class of models.
- For this reason, linear models were the go-to applied predictive modeling tool for decades,
- even though it usually meant giving up a couple points on the accuracy scale.
- These models will be referred to here as 'linear and monotonic',
- meaning that for a change in any given independent variable, the response function changes at a defined rate,
- in only one direction, and at a magnitude represented by a readily available coefficient

- Most machine learning algorithms create nonlinear, non-monotonic response functions.
- This class of functions is the most difficult to interpret, as they can change in a positive and negative direction and at a varying rate for any change in an independent variable.
- Typically, the only standard interpretability measure these functions provide are relative variable importance measures



Features

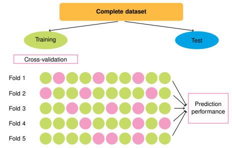
- variables used for model training.
- using the right features is crucial.

- More is not necessarily better (overfitting)!

- feature selection
- feature extraction/ engineering

- Machine learning uses so called features (i.e. variables or attributes) to generate predictive models
- Using a suitable combination of features is essential for obtaining high precision and accuracy.
- Because too many (unspecific) features pose the problem of overfitting the model, we generally want to restrict the features in our models to those, that are most relevant for the response variable we want to predict.
- Using as few features as possible will also reduce the complexity of our models, which means it needs less time and computer power to run and is easier to understand.
- Sometimes extraction of salient structure in the data that is more informative than the raw data itself (the feature extraction problem)

Training, (cross-) validation and test data



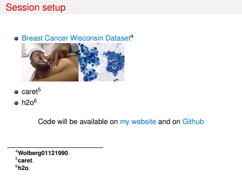
Decide cross validation strategy - To avoid overfitting, make sure you’ve set up a cross validation strategy in early stages. A nice CV strategy will help you get reliable score on leaderboard.

preventing overfitting, we want our models to be generalizable

Cross validation means that from my main set, I create RANDOMLY 2 sets. I built (train) my algorithm with the first one (let?s call it training set) and score the other (let?s call it validation set). I repeat this process multiple times and always check how my model performs on the test set in respect to the metric I want to optimize.

The process may look like:

For 10 (you choose how many X) times Split the set in training (50And validation (50Then fit the algorithm on the training set Score the validation set. Save the result of that scoring in respect to the chosen metric. Calculate the average of these 10 (X) times. That how much you expect this score in real life and is generally a good estimate. Remember to use a SEED to be able to replicate these X splits Other things to consider is Kfold and stratified KFold . Read here. For time sensitive data, make certain you always the rule of having past predicting future when testings.



Session setup

- Breast Cancer Wisconsin Dataset[4]
- caret[5]
- h2o[6]

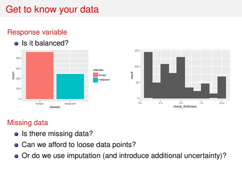
Code will be available on my website and on Github

[4] Wolberg01121990.
[5] caret.
[6] h2o.

- This breast cancer databases was obtained from the University of Wisconsin Hospitals, Madison
- from Dr. William H. Wolberg

- It looks at the predictor classes:
- malignant or
- benign breast mass

- The features characterise cell nucleus properties
- and were generated from image analysis of fine needle aspirates (FNA) of breast masses:
- Sample ID (code number)
- Clump thickness
- Uniformity of cell size
- Uniformity of cell shape
- Marginal adhesion
- Single epithelial cell size
- Number of bare nuclei
- Bland chromatin
- Number of normal nuclei
- Mitosis
- Classes, i.e. diagnosis



Get to know your data

Response variable

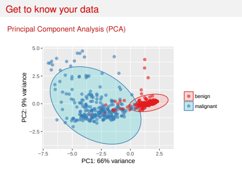
- Is it balanced?

Missing data

- Is there missing data?
- Can we afford to loose data points?
- Or do we use imputation (and introduce additional uncertainty)?

- Understand the data
- Look at data types.
- Check variable classes.
- Create some univariate - bivariate plots to understand the nature of variables.
- Most important to know is the distribution: are the classes balanced?
- If we have unbalanced data, this will effect our model later on
  We would have to consider over- or undersampling.

- Missing data
- If we have lots of data and few missing values, we can afford to loose these data points.
- If we don't have that much data though, our model will probably loose significant power if we remove the samples.
- In that case, we would rather introduce a certain uncertainty by imputing missing values.

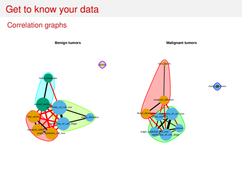


Get to know your data

Principal Component Analysis (PCA)

- Most real data sets are hard to see because they have many variables and many rows
- visualization can help when we reduce the complexity
- There are many techniques for projecting the rows of a data set from a usually high-dimensional original space into a more visually understandable lower-dimensional space:
- Principal Component Analysis (PCA)
- Multidimensional Scaling (MDS)
- t-distributed Stochastic Neighbor Embedding (t-SNE)
- Each of these techniques has strengths and weaknesses, but the key idea they all share is to represent the rows of a data set in a meaningful low-dimensional space.

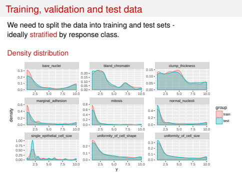
- To get an idea about the dimensionality and variance of the datasets, I am first looking at PCA plots
- for samples and features
- Principal component analysis (PCA) is a statistical procedure that uses an orthogonal transformation ...
- ... to convert a set of observations into a set of values of linearly uncorrelated variables called principal components
- The first two principal components (PCs) show the two components that explain the majority of variation in the data



Get to know your data

Correlation graphs

- A correlation graph is a two-dimensional representation of the relationships (correlation) in a data set
- Pearson correlation coefficient between features
- node size: sum of correlation coefficients
- edge width: correlation coefficient

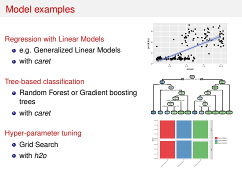


Training, validation and test data

We need to split the data into training and test sets - ideally stratified by response class.

Density distribution

For accurate predictions, density distribution should be similar in training and test data!



Model examples

Regression with Linear Models

- e.g. Generalized Linear Models
- with *caret*

Tree-based classification

- Random Forest or Gradient boosting trees
- with *caret*

Hyper-parameter tuning

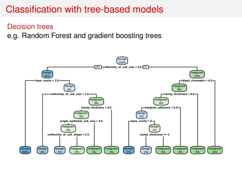
- Grid Search
- with *h2o*

There are over 250 ML algorithms implemented with caret alone. I am going to focus on two of the most widely used.

- traditional linear models tend to create linear, monotonic, and continuous functions
- Even though they?re not always the most accurate predictors, the elegant simplicity of linear models makes the results they generate easy to interpret.

- Of course, you need quite a bit of experience and intuition to hit on a good combination of parameters.
- That's why it usually makes sense to do a grid search for hyper-parameter tuning.
- Hyper-parameter tuning with grid search allows us to test different combinations of hyper-parameters and find one with improved accuracy.
- We can use the h2o.grid() function to perform a Random Grid Search (RGS). We could also test all possible combinations of parameters with Cartesian Grid or exhaustive search, but RGS is much faster when we have a large number of possible combinations and usually finds sufficiently accurate models.
- Based on the results of each model tested in the grid, we can choose the one with the highest accuracy or best performance for the question on hand

Classification with tree-based models



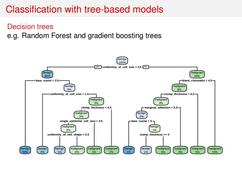
Classification with tree-based models

Decision trees

e.g. Random Forest and gradient boosting trees

- We start with a group of samples
- for each sample, we assign a class: e.g. it comes from a benign or malignant tumor
- for each sample, we also have a number of features
- a decision trees separates the data at several nodes to end up with classifications at the final leaves
- the model learns a conditional structure of discriminative features

- Random Forests produces multiple decision trees
- with some level of randomness
- Every node in the decision trees is a condition on a single feature, designed to split the dataset into two so that similar response values end up in the same set
- each tree is evaluated regarding how well it classified the samples (cross-validation)
- ensemble of all trees is used for prediction
- better generalization than individual trees



Classification with tree-based models

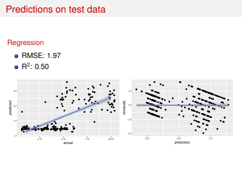
Decision trees

e.g. Random Forest and gradient boosting trees

- Not all of the features I created will be equally important to the model.
- A benefit of using ensembles of decision tree methods is that they can automatically provide estimates of feature importance from a trained predictive model.
- Generally, importance provides a score that indicates how useful or valuable each feature was in the construction of the decision trees within the model.
- The more an attribute is used to make key decisions with decision trees, the higher its relative importance.
- Importance is calculated for a single decision tree by the amount that each attribute split point improves the performanc measure, weighted by the number of observations the node is responsible for.
- The feature importances are then averaged across all of the the decision trees within the model.
- when training a tree, it can be computed how much each feature decreases the weighted impurity in a tree. For a fores the impurity decrease from each feature can be averaged and the features are ranked according to this measure.
- ’information gain’ is the measure that tells us how good a tree model is
- the measure based on which the (locally) optimal condition is chosen is called impurity. For classification, it is typically either Gini impurity or information gain/entropy and for regression trees it is variance

Never use the same data for evaluation that you used for training!

- Golden Rule of ML: always test model performance on indepenent data
- otherwise you will get overly optimistic performance measures
- The ultimate performance test for our model will be it’s prediction accuracy on the test set it hasn’t seen before.



Predictions on test data

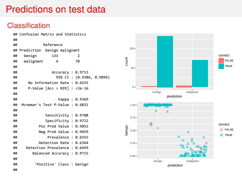
Regression

- RMSE: 1.97
- R^2: 0.50

- Residuals refer to the difference between the recorded value the predicted value
- Generally, the residuals of a well-fit model should be randomly distributed because good models will account for most phenomena in a data set, except for random error.

- In regression analysis, the term mean squared error refers to the unbiased estimate of error variance:
- the residual sum of squares divided by the number of degrees of freedom
- RMSE is a commonly used error metric to measure the performance of regression models.
- in regression the predictor variable is a real number, therefore to measure the quality of the predicted value from some algorithm you need to find some sort of difference between them. You do this by calculating the square of the error, tak the mean across all test objects and take square root
- A small RMSE means good prediction and large means bad model.
- RMSE is strongly influenced by outliers!

- R-squared is the ratio of explained variance to the total variance.
- it is a measure of how much of the variance in y is explained by the model. If R2 is close to one, then the model?s predictions mirror true outcome



Predictions on test data

Classification

```
## Confusion Matrix and Statistics
##
##            Reference
## Prediction  benign malignant
##   benign       133         2
##   malignant      4        70
##
##                Accuracy : 0.9713
##                  95% CI : (0.9386, 0.9894)
##     No Information Rate : 0.6555
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9369
##  Mcnemar's Test P-Value : 0.6831
##
##             Sensitivity : 0.9708
##             Specificity : 0.9722
##          Pos Pred Value : 0.9852
##          Neg Pred Value : 0.9459
##              Prevalence : 0.6555
##          Detection Rate : 0.6364
##    Detection Prevalence : 0.6459
##       Balanced Accuracy : 0.9715
##
##        'Positive' Class : benign
##
```

- precision == positive predictive value: fraction of predictions that are correct
- positive and negative predictive values: proportions of true positive and true negative results, depend on prevalence
- prevalence: how often each category occurs in the population
- recall == sensitivity == True Positive Rate: proportion of positives that are correctly identified (e.g., the percentage of si people who are correctly identified as having the condition).
- Specificity == True Negative Rate: proportion of negatives that are correctly identified (e.g., the percentage of healthy people who are correctly identified as not having the condition)
- Inverse Precision and Recall: Precision and Recall where positive and negative labels are exchanged
- detection rate == sensitivity

- Accuracy: weighted arithmetic mean of Precision and Recall
- Given a confusion matrix of classification results, the accuracy can be a misleading performance measure. Specifically, may falsely suggest above-chance generalizability:
- in binary classification, a training set consisting of different numbers of representatives from either class may result in a classifier that is biased towards the more frequent class
- this classifier may yield an optimistic accuracy estimate
- Balanced accuracy: average accuracy obtained on either class. Based on a confusion matrix

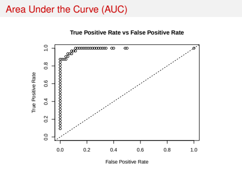
- p-value: one-sided test to see if the accuracy is better than the "no information rate"
- No Information Rate: the proportion of classes that you would guess right if you randomly allocated them
- Kappa: can have values between -1 and 1. 1 or -1 show complete agreement, zero shows complete disagreement
- McNemar's test: statistical test applied to 2 x 2 contingency tables to determine whether the row and column marginal frequencies are equal

2017-03-28

Webinar for ISDS R Group

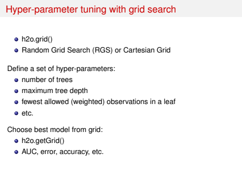
Evaluating model performance

Area Under the Curve (AUC)



Area Under the Curve (AUC)

- AUC usually refers to area under ROC curve (mathematically known as definite integral): Receiver Operating Characteristic
- metric for binary classification
- Accuracy deals with ones and zeros, meaning you either got the class label right or you didn?t. But many classifiers are able to quantify their uncertainty about the answer by outputting a probability value.
- From a random classifier you can expect as many true positives as false positives. That?s the dashed line on the plot.
- A score for a perfect classifier would be 1



Hyper-parameter tuning with grid search

- h2o.grid()
- Random Grid Search (RGS) or Cartesian Grid

Define a set of hyper-parameters:

- number of trees
- maximum tree depth
- fewest allowed (weighted) observations in a leaf
- etc.

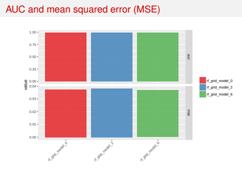
Choose best model from grid:

- h2o.getGrid()
- AUC, error, accuracy, etc.

We could also test all possible combinations of parameters with Cartesian Grid or exhaustive search, but RGS is much faster when we have a large number of possible combinations and usually finds sufficiently accurate models. For RGS, we first define a set of hyper-parameters and search criteria to fine-tune our models. Because there are many hyper-parameters, each with a range of possible values, we want to find an (ideally) optimal combination to maximize our model's accuracy. We can also specify how long we want to run the grid search for. Based on the results of each model tested in the grid, we can choose the one with the highest accuracy or best performance for the question on hand.

We now want to extract the best model from the grid model list. What makes a model *the best* depends on the question you want to address with it: in some cases, the model with highest AUC is the most suitable, or the one with the lowest mean squared error, etc. We first use the ‘h2o.getGrid()‘ function to sort all models by the quality metric we choose (depending on the metric, you want it ordered by descending or ascending values). We can then get the model that's the first in the list to work with further. This model's hyper-parameters can be found with ‘best model@allparameters‘. You can now work with your best model as with any regular model in **h2o**.

AUC and mean squared error (MSE)


AUC and mean squared error (MSE)

In statistics, the mean squared error (MSE) or mean squared deviation (MSD) of an estimator (of a procedure for estimating an unobserved quantity) measures the average of the squares of the errors or deviations?that is, the difference between the estimator and what is estimated. MSE is a risk function, corresponding to the expected value of the squared error loss or quadratic loss. The difference occurs because of randomness or because the estimator doesn't account for information that could produce a more accurate estimate.[1]

The MSE is a measure of the quality of an estimator?it is always non-negative, and values closer to zero are better. The MSE is the second moment (about the origin) of the error, and thus incorporates both the variance of the estimator and its bias. For an unbiased estimator, the MSE is the variance of the estimator. Like the variance, MSE has the same units of measurement as the square of the quantity being estimated. In an analogy to standard deviation, taking the square root of MSE yields the root-mean-square error or root-mean-square deviation (RMSE or RMSD), which has the same units as the quantity being estimated; for an unbiased estimator, the RMSE is the square root of the variance, known as the standard deviation.

The MSE assesses the quality of an estimator (i.e., a mathematical function mapping a sample of data to a parameter of the population from which the data is sampled) or a predictor (i.e., a function mapping arbitrary inputs to a sample of values of some random variable). Definition of an MSE differs according to whether one is describing an estimator or a predictor.

Grid Search

Start hyper parameter tuning - Once CV is at place, try improving model's accuracy using hyper parameter tuning. It further includes the following steps: Data transformations: It involve steps like scaling, removing outliers, treating null values, transform categorical variables, do feature selections, create interactions etc. Choosing algorithms and tuning their hyper parameters: Try multiple algorithms to understand how model performance changes. Saving results: From all the models trained above, make sure you save their predictions. They will be useful for ensembling. Combining models: At last, ensemble the models, possibly on multiple levels. Make sure the models are correlated