Models in Machine Learning

An Overview

LINEAR MODEL – FUNCTIONALITY

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General idea

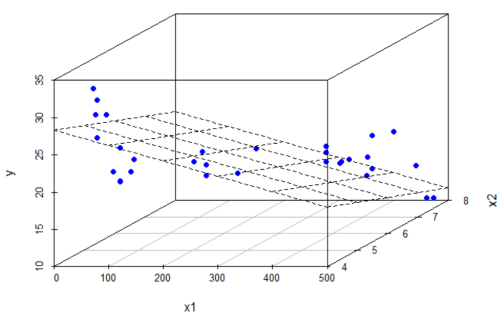
A linear model (LM) represents the target as a linear combination of the input variables.

Hypothesis space

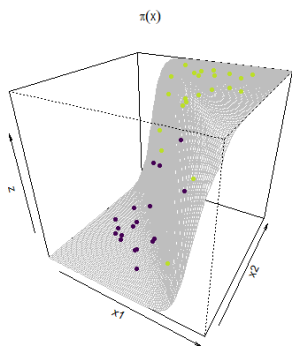
$\mathcal{H} = \left\{ f : \mathcal{X} \to \mathbb{R} \mid f(\mathbf{x}) = \phi(\boldsymbol{\theta}^\top \mathbf{x}) \right\}$, where $\phi(\cdot)$ is a transformation function.

For different $\phi(\cdot)$ it results in different models, e.g.:

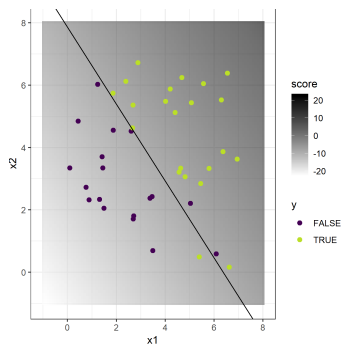
- identity function $\phi(\boldsymbol{\theta}^\top \mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x}$: **linear regression**
  models a continous output with the linear combination of the features $\boldsymbol{\theta}^T \mathbf{x}$.
- logistic sigmoid function $\phi(\boldsymbol{\theta}^\top \mathbf{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^\top \mathbf{x})} = \pi(\mathbf{x})$: **logistic regression**
  models a probability $\pi(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x})$ belonging to one of two classes.
  Applying a decision rule (e.g., $\pi(\mathbf{x}) > 0.5$) results in a separating hyperplane.



Linear regression: surface



Logisitc regression: surface



Logistic regression: classification

LINEAR MODEL – FUNCTIONALITY

Empirical risk

- Typically, in **linear regression** the **ordinary least squares (OLS)** with a squared loss function is used for regression: $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2$
- Alternatively, the **absolute loss** or the **Huber loss** can be used.
- For **logistic regression** the risk function is based on the **Bernoulli loss** $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} -y^{(i)} \log \left(\pi \left(\mathbf{x}^{(i)} \right) \right) - (1 - y^{(i)}) \log \left(1 - \pi \left(\mathbf{x}^{(i)} \right) \right)$.

Optimization

- for **OLS**: analytically with $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$
  (with $\mathbf{X} \in \mathbb{R}^{n \times p}$: matrix of feature vectors)
- for **other loss functions**: numerical optimization

Hyperparameters

None

LINEAR MODEL – PRO'S & CON'S

Advantages

+ **simple and fast** implementation; cheap computational costs
+ intuitive **interpretability**: mean influence of features on the output and feature importance
+ fits **linearly** separable data sets very well
+ works well **independent of data size**
+ basis for many machine learning algorithms

Disadvantages

- not suitable for data based on a **non-linear** data generating process $\rightarrow$ **strong simplification** of real-world problems
- **strong assumptions**: data is independent (multi-collinearity must be removed)
- tend to **overfit** (can be reduced by regularization)
- **sensitive to outliers and noisy data**

Simple method with good interpretability for linear problems, but strong assumptions and simplification of real-world problems

LINEAR MODEL – PRACTICAL HINTS

Check assumptions??

This model is very effective if the following assumptions are fulfilled:

- **linearity**: The expected response is a linear combination of the features.
- **homoscedasticity**: The variance of residuals is equal for all features.
- **independence**: All observations are independent of each other.
- **normality**: Y is normally distributed for any fixed value of the features

Implementation

- **R:** `mlr3` learner `LearnerRegrLM`, calling `stats::lm()`
- **Python:** `LinearRegression` from package `sklearn.linear_model`, package for advanced statistical parameters `statsmodels.api`

Regularization

In practice, we often use regularized models in order to **prevent overfitting** or perform feature selection. More details will follow in the subsequent chapter.

REGULARIZED LM – FUNCTIONALITY

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General idea

- Linear model (LM) can **overfit** if we operate in high-dimensional space with only a few observations.
- We can find a compromise between generalizing the model (simple model, underfitted) and corresponding closely to the data (complex model, overfitted).

Hypothesis space

$\mathcal{H} = \left\{ f : \mathcal{X} \to \mathbb{R} \mid f(\mathbf{x}) = \phi(\boldsymbol{\theta}^\top \mathbf{x}) \right\}$, where $\phi(\cdot)$ is a transformation function.

Empirical risk

- We minimize the empirical risk function $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ **plus a complexity penalty** $J(\boldsymbol{\theta})$, controlled by shrinkage parameter λ: $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \cdot J(\boldsymbol{\theta})$.
- **Ridge regression** uses the L2-penalty $J(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_2^2$.
- Alternativly, **LASSO** uses the L1-penalty $J(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_1$.

Optimization

- for **Ridge** regression: analytically with $\hat{\boldsymbol{\theta}}_{\text{Ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda \boldsymbol{I})^{-1}\mathbf{X}^T\mathbf{y}$
- for **LASSO regression**: e. g. (sub)-gradient descent

Hyperparameters

Shrinkage parameter λ

REGULARIZED LM – PRO'S & CON'S

ALMOST SAME LIKE LINEAR MODEL?–> does this make sense?

Advantages

+ simple and fast implementation; cheap computational costs
+ intuitive interpretability: mean influence of features on the output and feature importance
+ fits linearly separable data sets very well
+ works well independent of data size
+ basis for many machine learning algorithms
+ less tendency to **overfit**

Disadvantages

- not suitable for data based on a non-linear data generating process $\rightarrow$ strong simplification of real-world problems
- **strong assumptions**: data is independent (multi-collinearity must be removed and normal distributed residuals ??
- sensitive to outliers and noisy data

Simple method with good interpretability for linear problems, but strong assumptions and simplification of real-world problems.

REGULARIZED LM – PRACTICAL HINTS

Choice of regularization parameter λ

Choose λ with e. g. the smallest sum of squared residuals through cross-validation.
In the R package `glmnet` `lambda.min` is the value of λ that gives minimum mean cross-validated error.

Ridge vs. LASSO

- neither is overall better $\rightarrow$ elastic net as a compromise
- **Ridge** works better, if there are many influential and high correlated features.
- In contrast, **LASSO** is more suitable if the underlying structure is sparse (only a few features influence the output y).
- LASSO can set coefficients to zero, thus performing **variable selection**.

Implementation

- **R:** `mlr3` learners `LearnerClassifGlmnet` / `LearnerRegrGlmnet`, calling `glmnet::glmnet()`
- **Python:** `LinearRegression` from package `sklearn.linear_model`, package for advanced statistical parameters `statsmodels.api`

LINEAR SVM – FUNCTIONALITY

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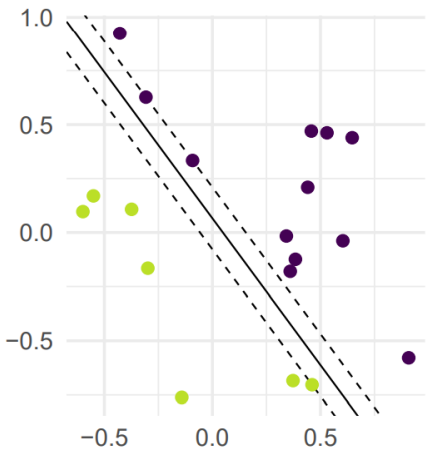
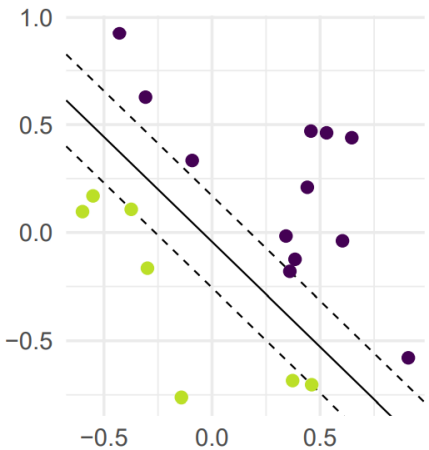
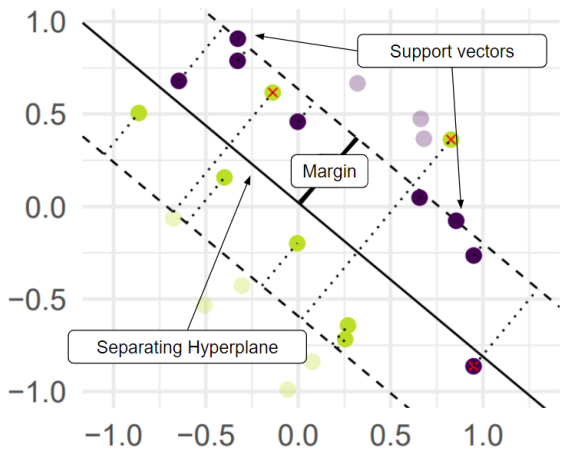
General idea

- The support vector machine (SVM) algorithm finds a decision boundary (**separating hyperplane**) that maximizes the distance (**margin** γ) to the closest members (**support vectors, SV**) of the separate classes. (**hard margin**)
- In a **soft-margin SVM** also "violations" of the margin are allowed $\rightarrow$ not only the margin should be maximized, but also the margin violations minimized.
- There are three different types of training points: **Non-SVs** which do not influence the hyperplane, **SVs** which are exactly on the hyperplane, and **margin violators**.

Hypothesis space $\mathcal{H} = \left\{ f : \mathcal{X} \to \mathbb{R} \mid f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x} + \theta_0 \right\}$







LINEAR SVM – FUNCTIONALITY

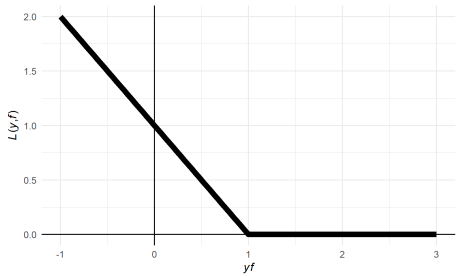
Empirical risk

Soft-margin SVMs can also be interpreted as **L2-regularized ERM**:

$$\frac{1}{2}\|\boldsymbol{\theta}\|^2 + C\sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

with $\|\boldsymbol{\theta}\| = 1/\gamma$,
C as a cost parameter for margin violation, and
$L(y, f)$ as the hinge loss.

$$L(y, f) = \max(1 - yf, 0),$$



Dual problem

$$\begin{aligned} \max_{\in\mathbb{R}^n} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} \left\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right\rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^{n} \alpha_i y^{(i)} = 0, \end{aligned}$$

Optimization **not differentiable** problem $\rightarrow$ mostly **subgradient** methods

Hyperparameters C : penalization for missclassified data points

LINEAR SVM – PRO'S & CON'S

Advantages

+ high **accuaracy**
+ often **sparse** solution
+ robust against overfitting (**regularized**); especially in high-dimensional space
+ **stable** solutions, as the non-SV do not influence the separating hyperplane

Disadvantages

- **costly implementation**; long training times
- does not scale well to **larger data sets ??**
- only **linear separation** $\rightarrow$ possible with non-linear SVMs which are explained in the following slides.
- poor **interpretability**

Very accurate solution for high-dimensional data that is linearly separable

LINEAR SVM – PRACTICAL HINTS

Preprocessing

Features must be rescaled before applying SVMs.

Tuning

The cost parameter C must be tuned, as it has a strong influence on the resulting separating hyperplane.

Implementation

- **R:** `mlr3` learners `LearnerClassifSVM` / `LearnerRegrSVM`, calling `svm()` from `libsvm`
- **Python:** `sklearn.svm.SVC` from package `scikit-learn` / package `libSVM`

NON-LINEAR SVM – FUNCTIONALITY

SUPERVISED | NON PARAMETRIC | BLACK-BOX

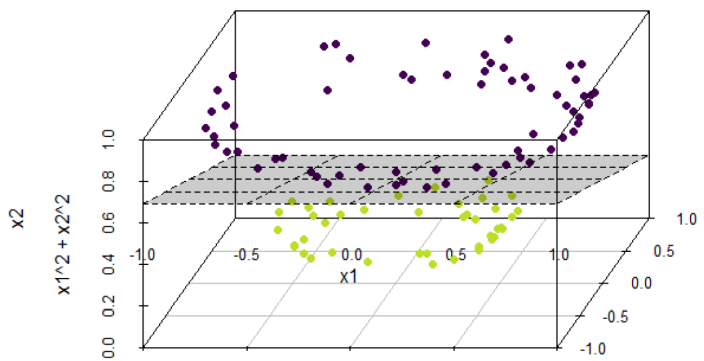
General idea

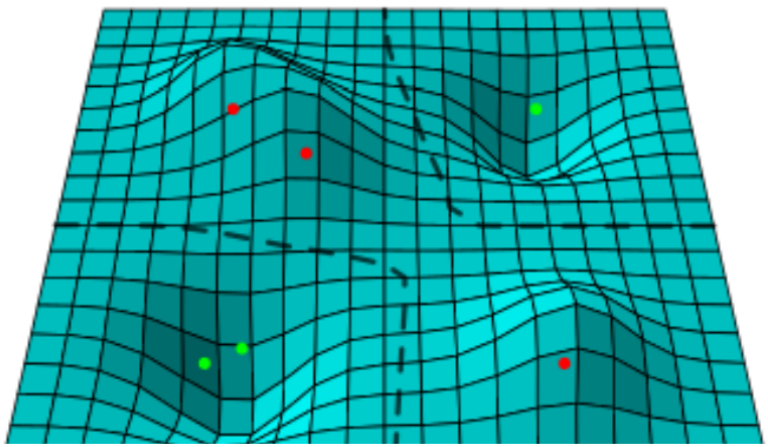
- Non-linear SVMs construct a separating hyperplane in a **higher dimensional dimension**
- **Kernels = feature map + inner product** $k(\mathbf{x}, \tilde{\mathbf{x}})$ transform the input space into a higher dimensional space and calculates the inner product.

Hypothesis space $\mathcal{H} = \{f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0 |\ \theta_0, \alpha_i \in \mathbb{R}\}$

$$\phi(x_1, x_2) = (x_1, x_2, x_1^2 + x_2^2)$$

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\gamma \|\mathbf{x} - \tilde{\mathbf{x}}\|^2)$$





NON-LINEAR SVM – FUNCTIONALITY

Dual Problem

We kernelize the dual (soft-margin) SVM problem by replacing all inner products $\left\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right\rangle$ by kernels $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$

$$
\begin{aligned}
\max_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \\
\text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\
& \sum_{i=1}^{n} \alpha_i y^{(i)} = 0.
\end{aligned}
$$

Hyperparameters

- C: penalization for missclassified data points
- **Kernel parameters**: depending on which kernel is used (e. g. degree of the polynomial kernel or width of RBF kernel)

NON-LINEAR SVM – PRO'S & CON'S

Advantages

+ high **accuaracy**
+ can learn **non-linear decision boundaries**
+ often **sparse** solution
+ robust against overfitting (**regularized**); especially in high-dimensional space
+ **stable** solutions, as the non-SV do not influence the separating hyperplane

Disadvantages

- **costly implementation**; long training times
- does not scale well to **larger data sets ??**
- only **linear separation** $\rightarrow$ possible with non-linear SVMs which are explained in the following slides.
- poor **interpretability**
- **not easy tunable** as it is highly important to choose the right kernel

Non-linear SVMs perform very well for non-linear separable data, but are hard to interpret and need a lot of tuning.

NON-LINEAR SVM – PRACTICAL HINTS

Kernels

Mainly, these three types of kernels are used:

- **Linear kernel**: the dot product of the given observations
- **Polynomial kernel**: curved lines in the input space
- **Radial basis function (RBF) kernel**: complex regions in the input space (e. g. spirals)

Tuning

- SVMs are sensitive to its hyperparameters and **should always be tuned**.
- For the RBF kernel the **RBF sigma heuristic** is used.

Implementation

- **R:** `mlr3` learners `LearnerClassifSVM` / `LearnerRegrSVM`, calling `e1071::svm()` (interface to `libSVM`)
- **Python:** `sklearn.svm.SVC` from package `scikit-learn` / package `libSVM`

K-NEAREST NEIGHBORS – FUNCTIONALITY

SUPERVISED | NON-PARAMETRIC | WHITE-BOX

General idea

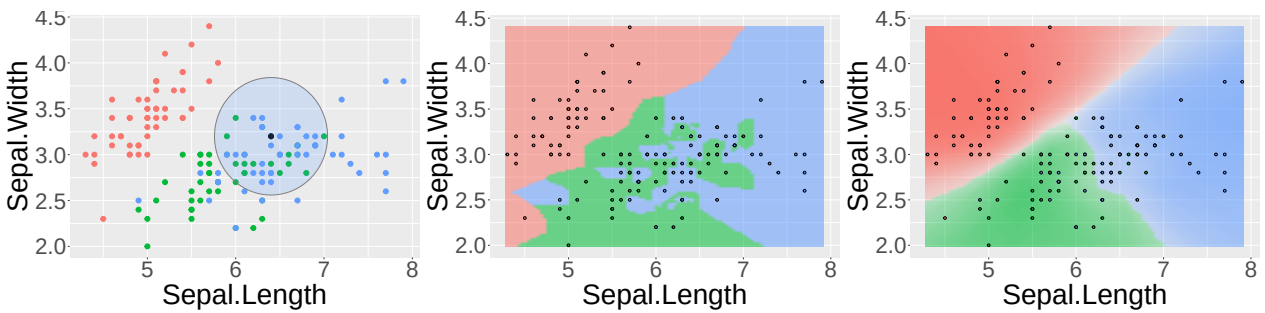
- The ***k*-nearest neighbors (*k*-NN)** model is based on inter-observational **distances**, thus heavily depending on the chosen **distance measure**.
- It builds upon the rationale that closeness in feature space infers closeness in target space.
- The prediction for $\mathbf{x}^{(i)}$ is the (weighted) **mean target** (regression) or **most frequent class** (classification) within its ***k*-neighborhood** $N_k(\mathbf{x}^{(i)})$ (i.e., the k points closest to $\mathbf{x}^{(i)}$ in feature space). only true for specific loss functions???

Hypothesis space $\mathcal{H} = \{f(\mathbf{x}) : f(\mathbf{x}) \text{ is a step function over a tesselation of } \mathcal{X}\}$

Empirical risk Any loss function applicable to regression/classification

Optimization Not necessary

Hyperparameters Neighborhood size k, distance measure $d(\cdot)$



Left: Neighborhood for exemplary observation in `iris`, $k = 50$
Right: Prediction surfaces for $k = 1$ and $k = 50$

K-NEAREST NEIGHBORS – PRO'S & CON'S

Advantages

+ **Easy** to explain and implement
+ Few **assumptions** - therefore (in theory) able to model data situations of **arbitrary complexity**
+ No **training** period
+ Constant evolvement with **new data**
+ Ability to learn **non-linear** decision boundaries
+ No **optimization** required
+ Only one **hyperparameter** to tune

Disadvantages

- Sensitivity toward **noisy** or **irrelevant** features
- Bad performance when feature **scales** are not consistent with importance
- Sensitivity toward **outliers**
- No handling of **missing** data
- Bad with data **imbalances**
- Large **memory** consumption for distance computation

Easy and intuitive for small, well-behaved data sets, but not suitable for large-scale data with problematic features

K-NEAREST NEIGHBORS – PRACTICAL HINTS

Non-parametric behavior

- k-NN is a **lazy classifier** – its parameters are the training data; there is no real compression of information.
- The number of parameters is thus equal to the number of observations (which have to be stored for prediction!).

Distance measures

- For numerical features, typically **Manhattan** or **Euclidean** distance; in presence of categorical features, **Gower** distance might be considered.
- Can be **weighted** to account for different scales or importance of features.

Neighborhoods in higher dimensions

k-NN is vulnerable to the **curse of dimensionality**: in very high-dimensional feature spaces, finding meaningful neighborhoods may become difficult.

Implementation

- **R:** `mlr3` learners `LearnerClassifKKNN` / `LearnerRegrKKNN`, calling `kknn::kknn()`
- **Python:** `KNeighborsClassifier` / `KNeighborsRegressor` from package `scikit-learn`

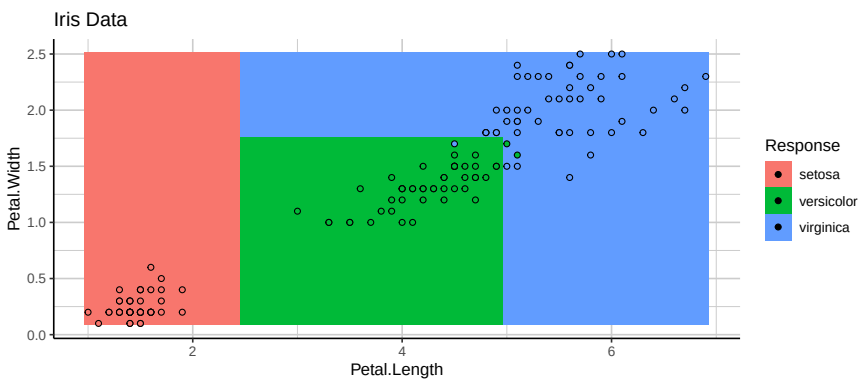
CART – FUNCTIONALITY

SUPERVISED | NON-PARAMETRIC | WHITE-BOX | FEATURE SELECTION

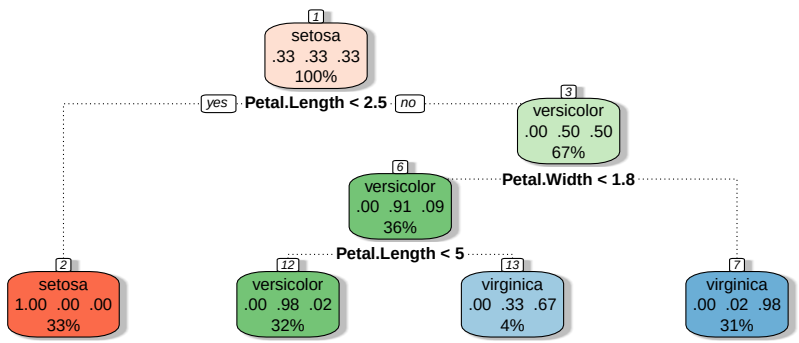
General idea

- Starting from a root node, **classification & regression trees (CART)** perform repeated **binary splits** of the data according to feature values, thereby subsequently dividing the input space $\mathcal{X}$ into T **rectangular partitions** Q_t.
- Observations are passed along until each ends up in exactly one leaf node (unless **stopped early** or **pruned**).
- In each step, CART find the optimal feature-threshold combination to split by.
- Leaf node t is assigned response c_t.

Hypothesis space $\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \sum_{t=1}^{T} c_t \mathbb{I}(\mathbf{x} \in Q_t) \right\}$



Prediction surface for `iris` data, 3 splits



Corresponding classification tree

CART – FUNCTIONALITY

Empirical risk

- Empirical risk is calculated for each potential terminal node $\mathcal{N}_t$ of a split.
- In general, trees can handle any type of loss function. Typical choices are:
  - Classification (for g classes):
    - Using **Brier score** $\mathcal{R}(\mathcal{N}_t) = \sum_{(\mathbf{x},y) \in \mathcal{N}_t} \sum_{k=1}^{g} \left(\mathbb{I}(y = k) - \pi_k(\mathbf{x})\right)^2$
    - Using **Bernoulli loss** $\mathcal{R}(\mathcal{N}_t) = \sum_{(\mathbf{x},y) \in \mathcal{N}_t} \sum_{k=1}^{g} \mathbb{I}(y = k) \cdot \log(\pi_k(\mathbf{x}))$
  - Regression: Using **quadratic loss** $\mathcal{R}(\mathcal{N}_t) = \sum_{(\mathbf{x},y) \in \mathcal{N}_t} (y - c_t)^2$

Optimization

Exhaustive search over all (randomly selected) split candidates in each node to minimize empirical risk in the child nodes (greedy optimization)

Hyperparameters

Complexity, i.e., number of leaves T

CART – PRO'S & CON'S

Advantages

+ **Easy** to understand, interpret & visualize
+ Automatic handling of **non-numerical** features
+ Built-in **feature selection**
+ Automatic handling of **missings**
+ **Interaction** effects between features easily possible, even of higher orders
+ **Fast** computation and good scalability
+ High **flexibility** (custom split criteria or leaf-node prediction rules)

Disadvantages

- Rather **low accuracy** (at least, without bagging or boosting)
- High **variance/instability**: strong dependence on training data
- Therefore, poor generalization & risk of **overfitting**
- Several steps required for modeling **linear** relationships
- In presence of categorical features, **bias** towards features with **many categories**

Simple and good with feature selection, but not the best predictor

CART – PRACTICAL HINTS

Pruning / early stopping

Unless interrupted, splitting will go on until each leaf node contains a single observation (expensive + overfitting!)

$\rightarrow$ Use **pruning** and **stopping criteria** to limit complexity

Implementation

- **R:** `mlr3` learners `LearnerClassifRpart` / `LearnerRegrRpart`, calling `rpart::rpart()`
- **Python:** `DecisionTreeClassifier` / `DecisionTreeRegressor` from package `scikit-learn`
- Complexity controlled via tree depth, minimum number of observations per node, maximum number of leaves, minimum risk reduction per split, ...

Bagging / boosting

Since CART are instable predictors on their own, they are typically ensembled to form a **random forest** (**bagging**) or used in combination with **boosting**.

RANDOM FOREST – FUNCTIONALITY

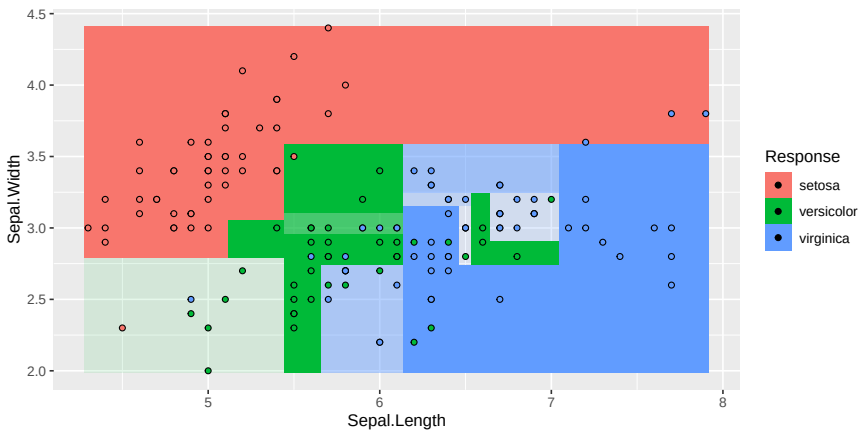
SUPERVISED | NON-PARAMETRIC | BLACK-BOX | FEATURE SELECTION

General idea

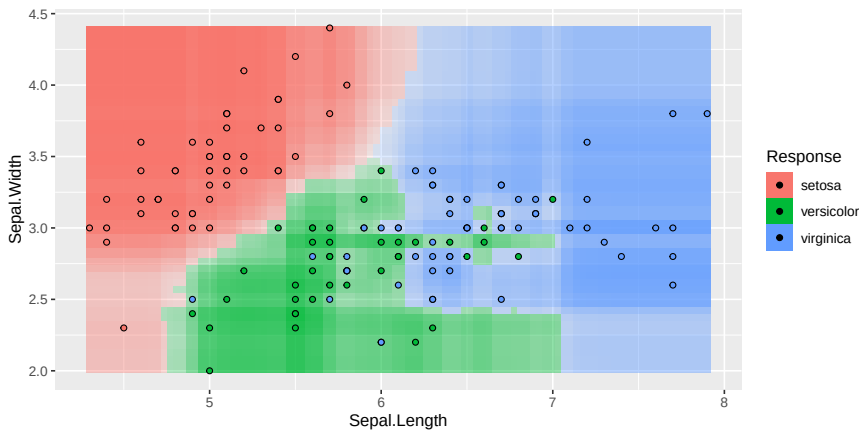
- **Random forests (RF)** perform **bagging**: they combine M trees (base learners) to form a strong **ensemble** learner.
- They use **complex** trees with low bias and compensate for the resulting variance by aggregating them in a **decorrelated** manner.
- Each tree is trained on a **bootstrap sample** of the data and only on a random **subset of features** to incur variability.
- Aggregation via **averaging** (regression) or **majority voting** (classification).

Hypothesis space

$$\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} \sum_{t=1}^{T^{[m]}} c_t^{[m]} \mathbb{I}(\mathbf{x} \in Q_t^{[m]}) \right\}$$



Prediction surface for `iris` data with a single tree



Prediction surface for `iris` data with 500-tree ensemble

RANDOM FOREST – FUNCTIONALITY

Empirical risk

- Applicable with **any** kind of loss function (just like tree base learners)
- Computation of empirical risk for all potential child nodes in all trees

Optimization

Exhaustive search over all (randomly selected) split candidates in each node of each tree to minimize empirical risk in the child nodes (greedy optimization)

Hyperparameters

- **Ensemble size**, i.e., number of trees
- **Complexity**, i.e., number of leaves T of each base learner
- **Number of split candidates**, i.e., number of features to be considered as splitting variables at each split
  $\rightarrow$ Frequently used heuristics: $\lfloor \sqrt{p} \rfloor$ for classification and $\lfloor p/3 \rfloor$ for regression

RANDOM FOREST – PRO'S & CON'S

Advantages

+ Translation of most of **base learners'** advantages (e.g., inherent variable selection, handling of missing data)
+ Fairly good at **prediction**: improved accuracy through bagging
+ Inherent computation of **feature importance**
+ Quite **stable** wrt changes in the data
+ Good with **high-dimensional** data, even in presence of noisy covariates
+ Applicable to **unbalanced** data
+ Easy to **parallelize**
+ Rather easy to **tune**

Disadvantages

- Translation of some of **base learners'** disadvantages (e.g., trouble to model linear relations, bias towards features with many categories)
- Loss of single trees' **interpretability** – black-box method
- Hard to **visualize**
- Often suboptimal for **regression**
- Often still inferior in **performance** to other methods (e.g., boosting)

Fairly good predictor, but black-box method

RANDOM FOREST – PRACTICAL HINTS

Pre-processing

Inherent feature selection of random forests, but high **computational costs** for large number of features

$\rightarrow$ Upstream feature selection (e.g., via PCA) might be advisable

Implementation

- **R:** `mlr3` learners `LearnerClassifRanger` / `LearnerRanger`, calling `ranger::ranger()`
- **Python:** `RandomForestClassifier` / `RandomForestRegressor` from package `scikit-learn`

Tuning

- Overall **limited tunability**
- Number of split candidates often more impactful than number of trees

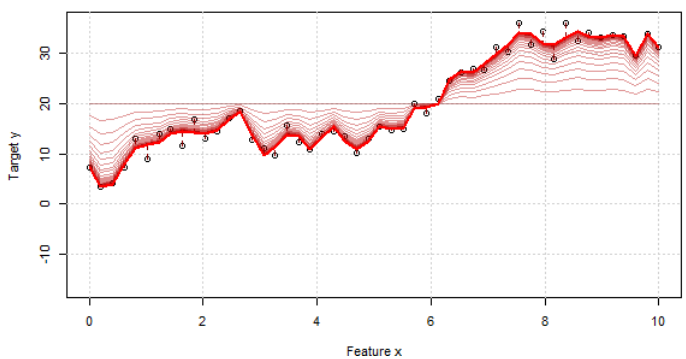
GRADIENT BOOSTING – FUNCTIONALITY

SUPERVISED | NON-PARAMETRIC | BLACK-BOX | FEATURE SELECTION

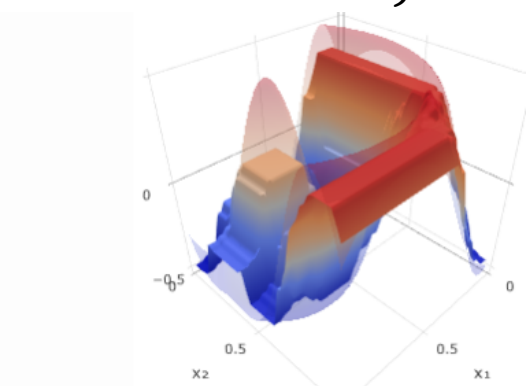
General idea

- **Gradient boosting (GB)** is an **ensemble** method that constructs a strong learner from weak base learners (frequently, CART).
- As opposed to **bagging**, however, base learners are assembled in a **sequential, stage-wise** manner: in each iteration, GB improves the current model by adding a new component that minimizes empirical risk.
- Each base learner is fitted to the current **point-wise residuals**
  $\rightarrow$ One boosting iteration $\widehat{=}$ one approximate **gradient step in function space**
- The final model is a weighted sum of base learners $b(\mathbf{x}, \theta^{[m]})$ with weights $\beta^{[m]}$.

Hypothesis space $\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \sum_{m=1}^{M} \beta^{[m]} b(\mathbf{x}, \theta^{[m]}) \right\}$



Gradient boosting for univariate function WHICH FIGURE



Gradient boosting for bivariate function WHICH FIGURE

GRADIENT BOOSTING – FUNCTIONALITY

Empirical risk

- **Outer loss:** Loss used to compute pseudo-residuals – how large is the error of the current model fit?
  $\rightarrow$ Arbitrary **differentiable** loss function
- **Inner loss:** Loss used to fit next base learner component to current pseudo-residuals
  $\rightarrow$ Typically, **quadratic loss** (desirable optimization properties)

Optimization **Functional gradient descent** for outer optimization loop, procedure for inner one depending on inner loss

Hyperparameters

- **Ensemble size**, i.e., number of base learners
- **Learning rate**, i.e., impact of single base learner
- **Complexity** of base learners (depending on type used)

GRADIENT BOOSTING – PRO'S & CON'S

Advantages

+ Powerful **off-the-shelf** method for supercharging weak learners' performance
+ Translation of most of **base learners'** advantages (e.g., for tree boosting: inherent variable selection, handling of missing data)
+ High predictive **accuracy** that is hard to outperform
+ High **flexibility** (custom loss functions, many tuning options)
+ Applicable to **unbalanced** data

Disadvantages

- Hardly **interpretable** – black-box method
- Hard to **visualize**
- Prone to **overfitting**
- Sensitive to **outliers**
- Hard to **tune** (high sensitivity to variations in hyperparameter values)
- Rather **slow** in training
- Hard to **parallelize**

High-performing predictor, but rather delicate to handle

GRADIENT BOOSTING – PRACTICAL HINTS

XGBoost (extreme gradient boosting)

Fast, efficient implementation of gradient-boosted decision trees that has become **state of the art** for many machine learning problems
$\rightarrow$ Clever modeling techniques + computational speed

Stochastic gradient boosting (SGB)

Faster, approximate version of GB that performs each iteration only on **random subset** of the data

Implementation

- **R:** `mlr3` learners `LearnerClassifXgboost` / `LearnerXgboost`, calling `xgboost::xgb.train()`
- **Python:** `GradientBoostingClassifier` / `GradientBoostingRegressor` from package `scikit-learn`, `XGBClassifier` / `XGBRegressor` from package `xgboost`

Tuning

- Overall **limited tunability**
- Number of split candidates often more impactful than number of trees

NEURAL NETWORK – FUNCTIONALITY

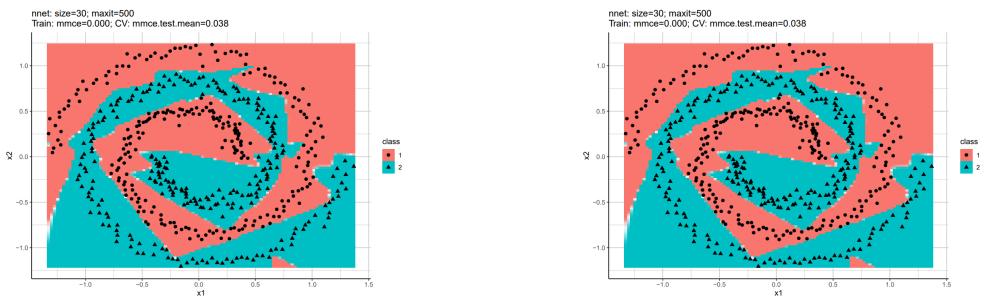
|UN| SUPERVISED | |NON| PARAMETRIC | BLACK-BOX

General idea

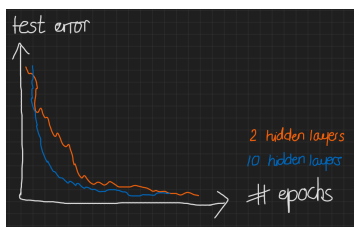
- A **neural network (NN)** is a model architecture loosely inspired by the human brain. It consists of various **neurons**, organized in **layers** assembled through weighted functional connections.
- Batches of data enter in the **input layer** and sequentially pass through h **hidden layers**, each of which performs a linear **transformation** $\phi^{(j)}$ and a non-linear **activation** $\sigma^{(j)}$, thus creating intermediary representations of the data.
- The **output layer** yields predictions after a final transformation ϕ and scaling τ.
- The resulting loss is used to update the weights for the next **epoch**.

Hypothesis space

$$\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \tau \circ \phi \circ \sigma^{(h)} \circ \phi^{(h)} \circ \sigma^{(h-1)} \circ \phi^{(h-1)} \circ \ldots \circ \sigma^{(1)} \circ \phi^{(1)}(\mathbf{x}) \right\}$$



Classification of `spirals` data with X & Y layers/epochs



Classification error vs layers/epochs

NEURAL NETWORK – FUNCTIONALITY

Empirical risk Any **differentiable** loss function

Optimization

NNs are optimized by **backpropagation** which consists of two steps:

- **Forward pass**: Predict result with current weights and compute empirical risk according to chosen loss function.
- **Backward pass**: Calculate error contribution of each weight by means of gradient descent – which essentially means applying the chain rule to the composition of functions applied in each layer – and update weights accordingly.

Hyperparameters

- Number of hidden **layers** (depth), number of **neurons** per layer
- **Activation** function(s)
- **Learning rate** for backpropagation
- Number of iterations (**epochs**), **batch** size
- Initial **weights**
- ...

NEURAL NETWORK – PRO'S & CON'S

Advantages

+ Able to solve **complex, non-linear** regression or classification problems
+ Therefore, typically very good **performance**
+ Built-in **feature extraction** - obtained by intermediary representations
+ Suitable for **unstructured** data (e. g. image, audio, text data)
+ Easy handling of **high-dimensional** or **missing** data
+ **Parallelizable** structure

Disadvantages

- Computationally **expensive** $\rightarrow$ slow to train and forecast
- Large **amounts** of data required
- **Faster-than-linear** scaling of weight matrices with increased network size
- Network architecture requiring much **expertise** in tuning
- **Black-box** model – hard to interpret or explain
- Tendency towards **overfitting**

Able to learn extremely complex functions, but computationally expensive and hard to get right

NEURAL NETWORK – PRACTICAL HINTS

Types of neural networks (RNNs, CNNs)

- **Recurrent neural networks (RNNs**: Deep NN that make use of **sequential** information with temporal **dependencies**
  $\rightarrow$ Frequently applied to **natural language processing**
- **Convolutional neural networks (CNNs)**: Regularized version of the fully connected feed-forward NN (where each neuron is connected to all neurons of the subsequent layer) that abstracts inputs to feature maps via **convolution**
  $\rightarrow$ Frequently applied to **image recognition**

Problem of neural architecture search (NAS)

NN are **not off-the-shelf** methods – the network architecture needs to be tailored to each problem anew
$\rightarrow$ Automated machine learning attempts to learn architectures

Implementation

- **R:** package `neuralnet`
- **Python:** libraries `PyTorch`, `keras`