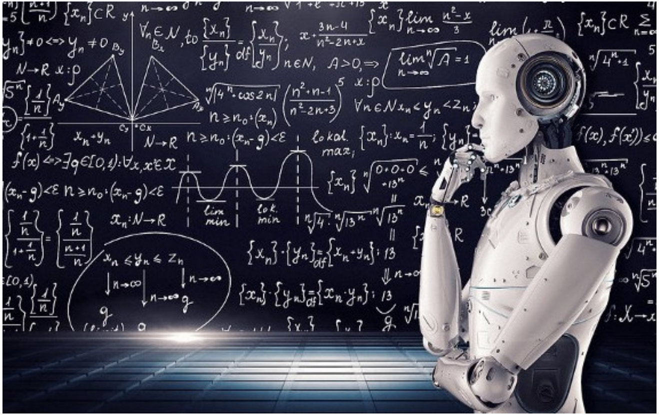
Common Machine Learning Algorithms



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LINEAR MODELS (LM)

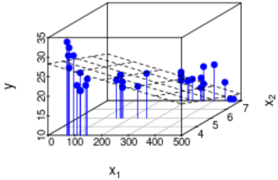
LINEAR MODELS – FUNCTIONALITY

REGRESSION | CLASSIFICATION | PARAMETRIC | WHITE-BOX

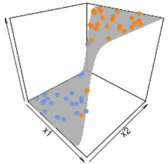
General idea Represent target as function of linear predictor $\boldsymbol{\theta}^T\mathbf{x}$

Hypothesis space $\mathcal{H} = \{f : \mathcal{X} \to \mathbb{R} \mid f(\mathbf{x}) = \phi(\boldsymbol{\theta}^\top\mathbf{x})\}$, with suitable transformation $\phi(\cdot)$, e.g.,

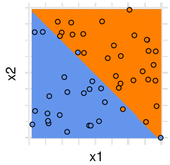
- Identity $\phi(\boldsymbol{\theta}^\top\mathbf{x}) = \boldsymbol{\theta}^\top\mathbf{x}$ $\Rightarrow$ **linear regression**
- Logistic sigmoid function $\phi(\boldsymbol{\theta}^T\mathbf{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^T\mathbf{x})} =: \pi(\mathbf{x} \mid \boldsymbol{\theta})$ $\Rightarrow$ **(binary) logistic regression**
  - Probability $\pi(\mathbf{x} \mid \boldsymbol{\theta}) = \mathbb{P}(y = 1 \mid \mathbf{x})$ of belonging to one of two classes
  - Separating hyperplane via decision rule (e.g., $\hat{y} = 1 \Leftrightarrow \pi(\mathbf{x}) > 0.5$)



Linear regression hyperplane



Logistic function for bivariate input and loss-minimal $\boldsymbol{\theta}$



Corresponding separating hyperplane

LINEAR MODELS – FUNCTIONALITY

Empirical risk

- **Linear regression**
  - Typically, based on **quadratic** loss: $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)^2$

    $\Rightarrow$ corresponding to ordinary-least-squares (OLS) estimation
  - Alternatives: e.g., **absolute** or **Huber** loss (both improving robustness)
- **Logistic regression:** based on **Bernoulli/log/cross-entropy** loss

  $\Rightarrow \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} -y^{(i)} \log\left(\pi\left(\mathbf{x}^{(i)}\right)\right) - (1 - y^{(i)}) \log\left(1 - \pi\left(\mathbf{x}^{(i)}\right)\right)$

Optimization

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

Hyperparameters None

LINEAR MODELS – PRO'S & CON'S

Advantages

+ **Simple and fast** implementation
+ **Analytical** solution
+ **Cheap** computation
+ Applicable for any **dataset size**, as long as number of observations $\gg$ number of features
+ Flexibility **beyond linearity** with polynomials, trigonometric transformations etc.
+ Intuitive **interpretability** via feature effects
+ Statistical hypothesis **tests** for effects available

Disadvantages

– **Nonlinearity** of many real-world problems
– Further restrictive **assumptions**: linearly independent features, homoskedastic residuals, normality of conditional response
– **Sensitivity** w.r.t. outliers and noisy data (especially with L2 loss)
– Risk of **overfitting** in higher dimensions
– Reature **interactions** must be handcrafted, so higher orders practically infeasible
– No handling of **missing** data

Simple, highly interpretable method suited for linear problems, but with strong assumptions, practical limitations, and tendency to overfit

LINEAR MODELS – REGULARIZATION

Idea

- Unregularized LM: risk of **overfitting** in high-dimensional space with only few observations
- **Goal**: find compromise between model fit and generalization by adding **penalty term**

Regularized empirical risk

- Empirical risk function **plus complexity penalty** $J(\boldsymbol{\theta})$, controlled by shrinkage parameter $\lambda > 0$:
  $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) := \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \cdot J(\boldsymbol{\theta})$.
- Popular regularizers
  - **Ridge** regression: L2 penalty $J(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_2^2$
  - **LASSO** regression: L1 penalty $J(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_1$

Optimization under regularization

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

LINEAR MODELS – REGULARIZATION

Choice of regularization parameter

- Standard hyperparameter optimization problem
- E.g., choose λ with minimum mean cross-validated error (default in R package `glmnet`)

Ridge vs. LASSO

- **Ridge**
  - Overall smaller, but still dense $\boldsymbol{\theta}$
  - Suitable with many influential features present, handling correlated features by shrinking their coefficients equally
- **LASSO**
  - Actual variable selection
  - Suitable for sparse problems, ineffective with correlated features (randomly selecting one)
- Neither overall better – compromise: **elastic net**
  $\rightarrow$ weighted combination of Ridge and LASSO regularizers

LINEAR MODELS – PRACTICAL HINTS

Implementation

- **R:**
  - **Unregularized:** `mlr3` learner `LearnerRegrLM`, calling `stats::lm()` / `mlr3` learner `LearnerClassifLogReg`, calling `stats::glm()`
  - **Regularized:** `mlr3` learners `LearnerClassifGlmnet` / `LearnerRegrGlmnet`, calling `glmnet::glmnet()`
- **Python:** `LinearRegression` from package `sklearn.linear_model`, package for advanced statistical parameters `statsmodels.api`

LINEAR SUPPORT VECTOR MACHINES (SVM)

LINEAR SVM – FUNCTIONALITY

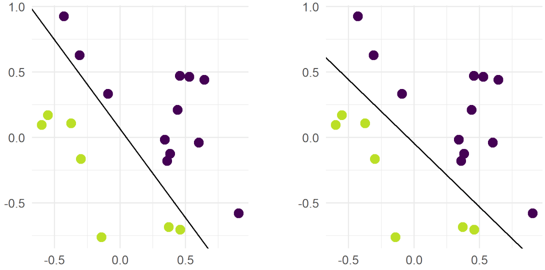
CLASSIFICATION PARAMETRIC BLACK-BOX

General idea

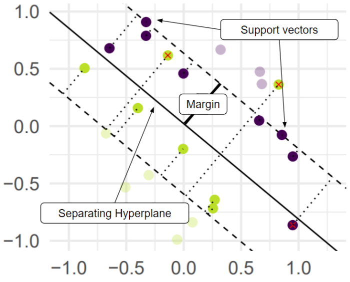
- Find linear decision boundary (**separating hyperplane**) that best separates classes
  - **Hard-margin** SVM: maximize distance (**margin** $\gamma > 0$) to closest members (**support vectors, SV**) on each side of decision boundary
  - **Soft-margin** SVM: relax separation to allowing margin violations $\rightarrow$ maximize margin while minimizing violations
- 3 types of training points
  - **non-SVs** with no impact on decision boundary
  - **SVs** located exactly on decision boundary
  - **margin violators**

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

LINEAR SVM – FUNCTIONALITY



Hard-margin SVM: margin is maximized by boundary on the right



Soft-margin SVM with margin violations

Dual problem

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^n} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n \alpha_i\alpha_j y^{(i)} y^{(j)} \left\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right\rangle$$

$$\text{s.t.} \quad 0 \leq \alpha_i \leq C \;\; \forall i \in \{1, \dots, n\} \;\; (C = \infty \text{ for hard-margin SVM}),$$

$$\sum_{i=1}^n \alpha_i y^{(i)} = 0$$

LINEAR SVM – FUNCTIONALITY

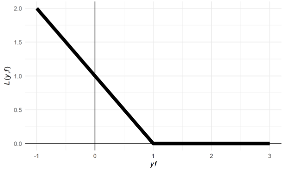
Empirical risk

Soft-margin SVM also interpretable 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

- $\|\boldsymbol{\theta}\| = 1/\gamma$,
- $C > 0$: penalization for missclassified data points
- $L(y, f) = \max(1 - yf, 0)$: **hinge** loss
  $\rightarrow$ other loss functions applicable (e.g., **Huber** loss)



Optimization

- Typically, tackling **dual** problem (though feasible in corresponding primal) via **quadratic programming**
- Popular: **sequential minimal optimization** $\rightarrow$ iterative algorithm based on breaking down objective into bivariate quadratic problems with analytical solutions

Hyperparameters Cost parameter C

LINEAR SVM – PRO'S & CON'S

Advantages

- + Often **sparse** solution
- + Robust against overfitting (**regularized**); especially in high-dimensional space
- + **Stable** solutions, as non-SV do not influence decision boundary

Disadvantages

- – **Costly** implementation; long training times
- – **Limited scalability** to larger data sets **??**
- – Confined to **linear separation**
- – Poor **interpretability**
- – No handling of **missing** data

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

LINEAR SVM – PRACTICAL HINTS

Preprocessing

Features must be rescaled before applying SVMs.

Tuning

Cost parameter C must be tuned and has strong influence on resulting separating hyperplane.

Implementation

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

NONLINEAR SUPPORT VECTOR MACHINES

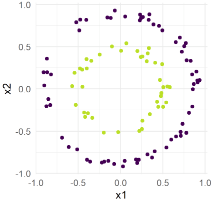
NONLINEAR SVM – FUNCTIONALITY

CLASSIFICATION | NONPARAMETRIC | BLACK-BOX

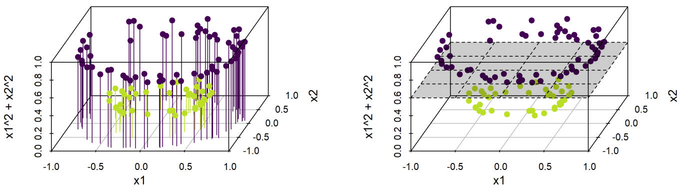
General idea

- Move **beyond linearity** by mapping data to transformed space where they are linearly separable
- **Kernel trick** (based on Mercer's theorem, existende of RKHS):
    - Replace two-step operation feature map $\phi \rightsquigarrow$ inner product by **kernel** $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, s.t. $\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}), =\rangle \, k(\mathbf{x}, \tilde{\mathbf{x}})$
    - No need for explicit construction of feature maps; very fast and flexible

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



Data are not linearly separable in original space.



Mapping to 3D space allows for linear separation with hyperplane.

NONLINEAR SVM – FUNCTIONALITY

Dual problem

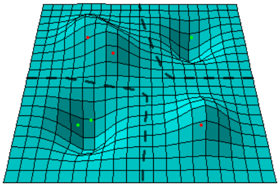
Kernelize dual (soft-margin) SVM problem, replacing all inner products $\left\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right\rangle$ by kernels:

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

Hyperparameters Cost C of margin violations, kernel hyperparameters (e.g., width of RBF kernel)

Interpretation as basis function approach

- **Representer theorem:** dual soft-margin SVM problem can be expressed through $\boldsymbol{\theta} = \sum_{j=1}^{n} \beta_j \phi\left(\mathbf{x}^{(j)}\right)$
- Sparse, weighted sum of **basis functions** with $\beta_j = 0$ for non-SVs
- **Local** model with smoothness depending on kernel properties



RBF kernel as mixture of Gaussian basis functions, forming bumpy, nonlinear decision surface to discern red and green points.

NONLINEAR SVM – PRO'S & CON'S

Advantages

- + high **accuaracy**
- + can learn **nonlinear 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** → possible with nonlinear SVMs which are explained in the following slides.
- – poor **interpretability**
- – **not easy tunable** as it is highly important to choose the right kernel
- – No handling of **missing** data

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

NONLINEAR SVM – PRACTICAL HINTS

Popular kernels

- **Linear** kernel: dot product of given observations $\rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x}^\top \tilde{\mathbf{x}}$
- **Polynomial** kernel of degree $d \in \mathbb{N}$: monomials (i.e., feature interactions!) up to d-th order $\rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \left(\mathbf{x}^\top \tilde{\mathbf{x}} + b\right)^d, \ b \geq 0$
- **RBF** kernel: infinite-dimensional feature space, in theory allowing for perfect separation of all finite datasets $\rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\gamma \|\mathbf{x} - \tilde{\mathbf{x}}\|_2^2\right)$ with bandwidth parameter $\gamma > 0$

Tuning

- High sensitivity w.r.t. hyperparameters, especially those of kernel $\rightarrow$ **tuning** very important
- For RBF kernels, use **RBF sigma heuristic** to determine bandwidth

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 (K-NN)

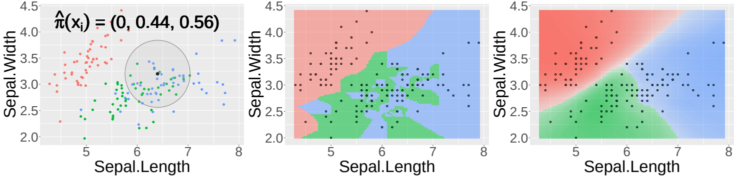
K-NN – FUNCTIONALITY

REGRESSION | CLASSIFICATION | NONPARAMETRIC | WHITE-BOX

General idea

- Rationale: **similarity** in feature space $\rightsquigarrow$ similarity in target space w.r.t. some similarity/distance **metric**
- **Prediction** for $\mathbf{x}$: construct k**-neighborhood** $N_k(\mathbf{x})$ from k points closest to $\mathbf{x}$ in $\mathcal{X}$, then predict
  - (weighted) mean target for **regression**: $\hat{y} = 1/\left(\sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} w_i\right) \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} w_i y^{(i)}$
  - most frequent class for **classification**: $\hat{y} = \arg\max_{\ell \in \{1, \ldots, g\}} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$
- No distributional or functional **assumptions**
- **Nonparametric** behavior: parameters = training data; no compression of information

Hyperparameters Neighborhood **size** k (locality), **distance** measure



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

K-NN – PRO'S & CON'S

Advantages

+ **Easy** to explain and implement
+ Applicable to both regression and classification tasks
+ No functional **assumptions** – therefore (in theory) able to model data situations of **arbitrary complexity**
+ No **training** period; no **optimization** required
+ Constant evolvement with **new data**
+ Ability to learn **non-linear** decision boundaries

Disadvantages

– Sensitivity w.r.t. **noisy** or **irrelevant** features and outliers due to utter reliance on distances
– Bad performance when feature **scales** not consistent with importance
– Heavily afflicted by **curse of dimensionality**
– No handling of **missing** data
– Poor handling of data **imbalances** (worse for large k)
– High **memory** consumption of distance computation

Easy and intuitive for small, well-behaved datasets with meaningful feature space distances

K-NN – PRACTICAL HINTS

Popular distance measures

- Numerical features: typically, **Minkowski** distances $d(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|_q = \left(\sum_j |x_j - \tilde{x}_j|^q\right)^{\frac{1}{q}}$
  - $q = 1$: **Manhattan** distance $\rightarrow d(\mathbf{x}, \tilde{\mathbf{x}}) = \sum_j |x_j - \tilde{x}_j|$
  - $q = 2$: **Euclidean** distance $\rightarrow d(\mathbf{x}, \tilde{\mathbf{x}}) = \sqrt{\sum_j (x_j - \tilde{x}_j)^2}$
- In presence of categorical features: **Gower** distance
- **Custom** distance measures applicable
- Optional **weighting** to account for beliefs about varying feature importance

Implementation

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

CLASSIFICATION & REGRESSION TREES (CART)

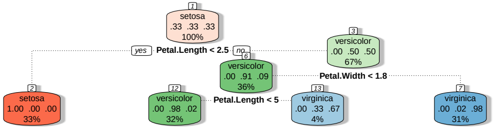
CART – FUNCTIONALITY

REGRESSION | CLASSIFICATION | NONPARAMETRIC | WHITE-BOX | FEATURE SELECTION

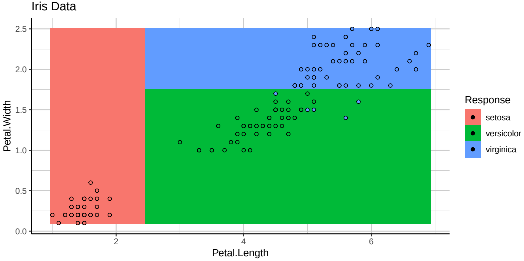
General idea

- Starting from root node containing all data, perform repeated **binary splits**, thereby subsequently dividing input space into T **rectangular partitions** Q_t
  - In each step, find **optimal split** (feature-threshold combination) $\rightarrow$ greedy search
  - Assign same response c_t to all observations in terminal region Q_t
- Splits based on node **impurity**, equivalently interpretable as **ERM**

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



Classification tree for `iris` data after 3 splits



Correspongincg prediction surface with axis-aligned boundaries

CART – FUNCTIONALITY

Empirical risk

- Calculated for each potential terminal node $\mathcal{N}_t$ of a split
- In general, compatible with arbitrary losses – typical choices:
  - g-way classification:
    - **Brier score** $\mathcal{R}(\mathcal{N}_t) = \sum_{(\mathbf{x}, y) \in \mathcal{N}_t} \sum_{k=1}^{g} (\mathbb{I}(y = k) - \pi_k(\mathbf{x}))^2 \quad \rightarrow$ **Gini** impurity
    - **Bernoulli** loss $\mathcal{R}(\mathcal{N}_t) = \sum_{(\mathbf{x}, y) \in \mathcal{N}_t} \sum_{k=1}^{g} \mathbb{I}(y = k) \cdot \log(\pi_k(\mathbf{x})) \quad \rightarrow$ **entropy** impurity
  - Regression: **quadratic** loss $\mathcal{R}(\mathcal{N}_t) = \sum_{(\mathbf{x}, y) \in \mathcal{N}_t} (y - c_t)^2$

Optimization

- **Exhaustive** search over all split candidates, choice of risk-minimal split
- In practice: limit number of candidates, use tricks to avoid combinatorial explosion

Hyperparameters **Complexity**, i.e., number of leaves T (controlled indirectly, see *Implementation*)

CART – PRO’S & CON’S

Advantages

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

Disadvantages

- — Rather **poor generalization** when used stand-alone
- — High **variance/instability**: strong dependence on training data
- — Substantial risk of **overfitting**
- — Not well-suited for modeling **linear** relationships
- — **Bias** toward features with **many categories**

Simple, good with feature selection and highly interpretable, but not the most performant learner

CART – PRACTICAL HINTS

Complexity control

- Unless interrupted, splitting continues until we have one observation per leaf node (costly + overfitting)
- Limit tree growth via
  - **Early stopping:** stop growth prematurely
    $\rightarrow$ hard to determine good stopping point before actually trying all combinations
  - **Pruning:** grow to large size and cut back in risk-optimal manner

Bagging / boosting As CART are highly **instable** predictors on their own, they are typically used as base learners in bagging (random forest) or boosting ensembles.

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, ...

RANDOM FORESTS

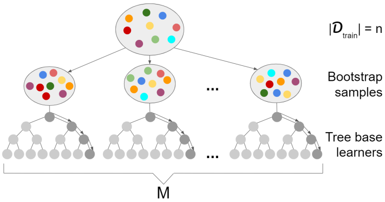
RANDOM FORESTS – FUNCTIONALITY

REGRESSION | CLASSIFICATION | NONPARAMETRIC | BLACK-BOX | FEATURE SELECTION

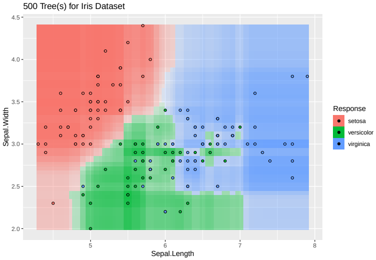
General idea

- Combine M tree **base learners** into **bagging ensemble**, fitting same learner on **bootstrap** data samples
  - Use unstable, **high-variance** base learners $\rightarrow$ let trees grow to full size
  - Mitigate invididual trees' bias by promoting **decorrelation** $\rightarrow$ use random subset of candidate features for each split
- **Prediction** via averaging (regression) or majority vote (classification)

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



Schematic depiction of bagging process



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

RANDOM FORESTS – 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 split candidates in each node of each tree to minimize empirical risk in child nodes (greedy optimization)

Hyperparameters

- **Ensemble size**, i.e., number of trees
- **Complexity** of base learners
- **Number of split candidates**, i.e., number of features to be considered at each split
  $\rightarrow$ frequently used heuristics with total of p features: $\lfloor \sqrt{p} \rfloor$ for classification, $\lfloor p/3 \rfloor$ for regression

Out-of-bag (OOB) error

- Compute ensemble prediction for observations outside individual trees' bootstrap training sample
  $\rightarrow$ unseen test points
- Use resulting loss as unbiased estimate of **generalization error**

RANDOM FORESTS – PRO'S & CON'S

Advantages

+ Translation of most of **trees'** advantages (e.g., feature selection, feature interactions)
+ Fairly good **good predictors**: mitigating base learners' weakness through bagging
+ Quite **stable** w.r.t. changes in data
+ Good with **high-dimensional** data, even in presence of noisy covariates
+ Easy to **parallelize**
+ Rather easy to **tune**
+ Intuitive measures of **feature importance**

Disadvantages

— Loss of trees' **interpretability** – black-box method

— Hard to **visualize**

— Often suboptimal for **regression**

— **Bias** toward features with **many categories**

— Often still inferior in **performance** to other methods (e.g., boosting)

Fairly good and stable predictor with built-in feature selection, but black-box method

RANDOM FORESTS – PRACTICAL HINTS

Pre-processing Inherent feature selection, but high **computational cost** for large number of features
$\rightarrow$ upstream feature selection (e.g., via PCA) might be advisable

Feature importance

- Based on **improvement in split criterion:** aggregate improvements by all splits using *j*-th feature
- Based on **permutation:** permute *j*-th feature in OOB observations and compute impact on OOB error

Tuning Number of split candidates often more impactful than number of trees

Implementation

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

GRADIENT BOOSTING

GRADIENT BOOSTING – FUNCTIONALITY

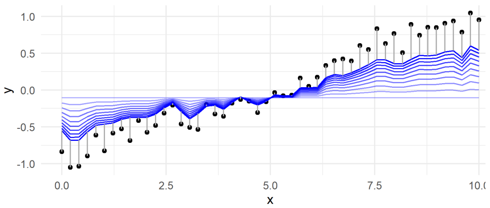
REGRESSION | CLASSIFICATION | (NON)PARAMETRIC | BLACK-BOX | FEATURE SELECTION

General idea

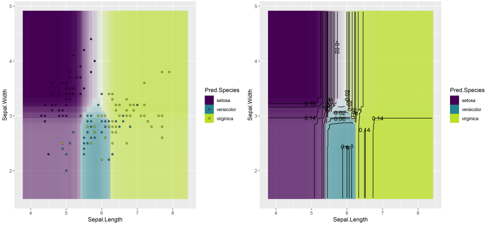
- Create **ensemble** in **sequential**, stage-wise manner
  - In each iteration, add new model component in risk-minimal fashion
  - Final model: weighted sum of base learners (frequently, **CART**)
- Fit each base learner to current **point-wise residuals**
  $\rightarrow$ one boosting iteration $\widehat{=}$ one approximate **gradient step in function space**

Hypothesis space

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



Boosting prediction function with GAM base learners for univariate regression problem after 10 iterations



Boosting prediction surface with tree base learners for `iris` data after 100 iterations (*right:* contour lines of discriminant functions)

GRADIENT BOOSTING – FUNCTIONALITY

Empirical risk

- **Outer loss** used to compute pseudo-residuals – error of current model fit?
  $\rightarrow$ arbitrary **differentiable** loss function
- **Inner loss** used to fit next base learner component to current pseudo-residuals
  $\rightarrow$ typically, **quadratic loss**

Optimization **Functional gradient descent** for outer optimization loop´

Hyperparameters

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

GRADIENT BOOSTING – PRO'S & CON'S

Advantages

- \+ Powerful **off-the-shelf** method for supercharging weak learners' performance
- \+ High predictive **performance** that is hard to outperform
- \+ Translation of most of **base learners'** advantages
- \+ High **flexibility** (custom loss functions, many tuning options)

Disadvantages

- — Hard to **interpret** – 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 and flexible predictor, but rather delicate to handle

GRADIENT BOOSTING – PRACTICAL HINTS

XGBoost (extreme gradient boosting)

- Fast, efficient implementation of gradient-boosted decision trees
- **State of the art** for many machine learning problems

Stochastic gradient boosting (SGB) Faster, approximate version of GB that performs each iteration only on **random data subset**

Tuning Tipps??

Implementation

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

NEURAL NETWORKS (NN)

NEURAL NETWORKS – FUNCTIONALITY

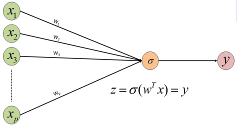
REGRESSION | CLASSIFICATION | (NON)PARAMETRIC | BLACK-BOX | FEATURE SELECTION

General idea

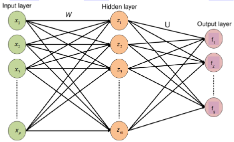
- Learn **composite function** through series of feature transformations, with components distributed over **neurons** organized in **layers**
  - Basic operation of each neuron: 1) affine **transformation**, 2) (nonlinear) **activation**
  - **Arbitrarily complex** combinations of fundamental building blocks
- Learning through **backpropagation**, performing alternating steps:
  - **Forward pass**: predict result with current parameters and compute empirical risk
  - **Backward pass**: update each parameter in proportion to its error contribution $\rightarrow$ gradients

Hypothesis space

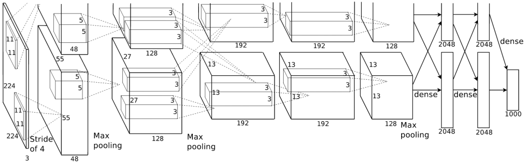
$$\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \tau \circ \phi \circ \sigma^{(h)} \circ \phi^{(h)} \circ \sigma^{(h-1)} \circ \phi^{(h-1)} \circ \ldots \circ \sigma^{(1)} \circ \phi^{(1)}(\mathbf{x}) \right\}$$



Single neuron



Feedforward network, 1 hidden layer



Convolutional network architecture

NEURAL NETWORKS – FUNCTIONALITY

Empirical risk Any **differentiable** loss function

Optimization

- Variety of different optimizers, most based on some form of **stochastic gradient descent**
- Backbone: gradient computation for arbitrary functions via **computational graphs**
- Crucial role of **regularization** due to high expressivity of NNs' hypothesis spaces

NN types Large variety of architectures for different purposes

- **Feedforward NNs** / **multi-layer perceptrons (MLPs):** sequence of **fully-connected** layers with all neurons linked to each other
- **Convolutional NNs (CNNs):** sequence of feature map extractors with spatial awareness $\rightarrow$ images
- **Recurrent NNs (RNNs):** handling of sequential, variable-length information with temporal dependencies $\rightarrow$ times series, text, audio
- **Autoencoders:** learning unsupervised embeddings
- **Generative adversarial networks (GANs):** learning to generate artificial samples

Hyperparameters

- Network **depth** (i.e., number of layers)
- Number of hidden **layers** (depth), number of **neurons** per layer
- **Activation** function(s)
- **Learning rate** for backpropagation

NEURAL NETWORKS – 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 NETWORKS – PRACTICAL HINTS

NN regularization dropout, batchnorm, lr scheduler, weight decay, ...

Optimizers

Implementation

- **R:** package `neuralnet`
- **Python:** libraries `PyTorch` and `PyTorch Lightning`, `TensorFlow` (high-level API: `keras`)