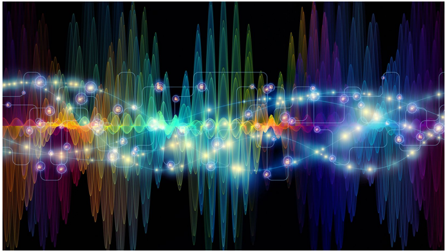
Common Machine Learning Algorithms



Learning goals

- Understand general idea of most important ML algorithms
- Learn to choose best-suited algorithm by weighing strengths and weaknesses
- Apply algorithms more effectively

CONTENTS

1 Linear Models (LM)

2 Linear Support Vector Machines (SVM)

3 Nonlinear Support Vector Machines

4 *k*-Nearest Neighbors (*k*-NN)

5 Classification & Regression Trees (CART)

6 Random Forests

7 Gradient Boosting

8 Neural Networks (NN)

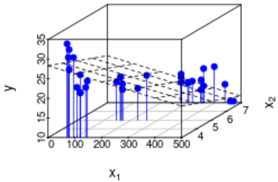
LINEAR MODELS – METHOD SUMMARY

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

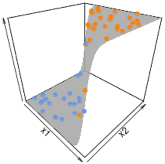
General idea Represent target as function of linear predictor $\boldsymbol{\theta}^T\mathbf{x}$ with interpretable effect coefficients $\boldsymbol{\theta}$

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.,

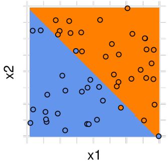
- Identity $\phi(\boldsymbol{\theta}^\top\mathbf{x}) = \boldsymbol{\theta}^\top\mathbf{x}$ $\rightarrow$ **linear regression**
- Logistic sigmoid function $\phi(\boldsymbol{\theta}^T\mathbf{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^T\mathbf{x})} =: \pi(\mathbf{x} \mid \boldsymbol{\theta})$ $\rightarrow$ **(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 – METHOD SUMMARY

Empirical risk

- **Linear regression**
  - Typically, based on **quadratic** loss: $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)^2 \quad \Rightarrow$ OLS estimation
- **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**: analytical solution $\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$, for other loss functions: numerical optimization

Multi-class extension of logistic regression

- Estimate **class-wise** scoring functions: $\Rightarrow \pi : \mathcal{X} \to [0,1]^g,\ \pi(\mathbf{x}) = (\pi_1(\mathbf{x}), \ldots, \pi_g(\mathbf{x})),\ \sum_{k=1}^{g} \pi_k(\mathbf{x}) = 1$
- Achieved through **softmax** transformation: $\pi_k(\mathbf{x}) = \exp(\boldsymbol{\theta}_k^\top \mathbf{x}) \Big/ \sum_{k=1}^{g} \exp(\boldsymbol{\theta}_j^\top \mathbf{x})$
- Multi-class log-loss: $L\left(y, \pi(\mathbf{x})\right) = -\sum_{j=1}^{g} \mathbb{I}_{\{y=k\}} \log(\pi_k(\mathbf{x}))$
- Predict class with maximum score (or use thresholding variant)

LINEAR MODELS – PRO'S & CON'S

Advantages

- + **Simple and fast** implementation
- + **Analytical** solution for quadratic loss
- + **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
- — Feature **interactions** must be handcrafted, so higher orders practically infeasible
- — No handling of **missing** data

Simple, highly interpretable method, but with strong assumptions, practical limitations, and risk of overfitting

LINEAR MODELS – REGULARIZATION

General 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**
- Regularization ubiquitous in ML, with similar techniques

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**
  - Global shrinkage, leading to overall smaller but still dense $\boldsymbol{\theta}$
  - Applicable with large number of influential features, handling correlated variables by shrinking their coefficients to equal degree
- **LASSO**
  - Actual variable selection by shrinking coefficients for irrelevant features all the way to zero
  - Suitable for sparse problems, ineffective with correlated features (randomly selecting one)
- Neither overall better $\Rightarrow$ compromise: **elastic net**
  - Weighted combination of Ridge and LASSO
  - Introducing additional penalization coefficient: $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda_1 \cdot \|\boldsymbol{\theta}\|_1 + \lambda_2 \cdot \|\boldsymbol{\theta}\|_2^2$

LINEAR MODELS – PRACTICAL HINTS

Implementation

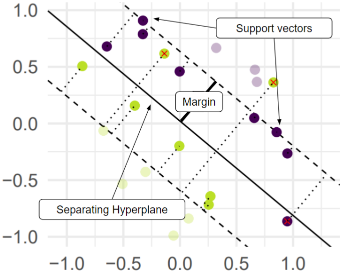
- **R:**
  - **Unregularized:** `mlr3` learner `LearnerRegrLM`, calling `stats::lm()` / `mlr3` learner `LearnerClassifLogReg`, calling `stats::glm()`
  - **Regularized:** `mlr3` learners `LearnerClassifGlmnet` / `LearnerRegrGlmnet`, calling `glmnet::glmnet()`
  - For **large classification** models: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

LINEAR SVM – METHOD SUMMARY

CLASSIFICATION REGRESSION PARAMETRIC WHITE-BOX

General idea

- Find linear decision boundary (**separating hyperplane**) that best discriminates classes
  - **Hard-margin** SVM: maximize distance (**margin** $\gamma > 0$) to closest points (**support vectors, SVs**) on each side of decision boundary
  - **Soft-margin** SVM: relax separation to allow for margin violations ⇒ 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**
- **Interpretable** weighted sum of basis functions with positive coefficients for support vectors
- Extension to **regression** is possible but requires modifications ⇒ here: only classification case



Soft-margin SVM with margin violations

Hypothesis space $\left\{ f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i y^{(i)} \langle \mathbf{x}^{(i)}, \mathbf{x} \rangle + \theta_0 \mid \theta_0, \alpha_i \in \mathbb{R} \, \forall i \right\}$

LINEAR SVM – METHOD SUMMARY

Dual problem Motivation: ...

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

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

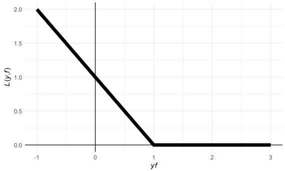
$$\sum_{i=1}^n \alpha_i y^{(i)} = 0$$

Empirical risk Soft-margin SVM also interpretable as **L2-regularized ERM**:

$$\frac{1}{2} \|\boldsymbol{\theta}\|_2^2 + C \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

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)



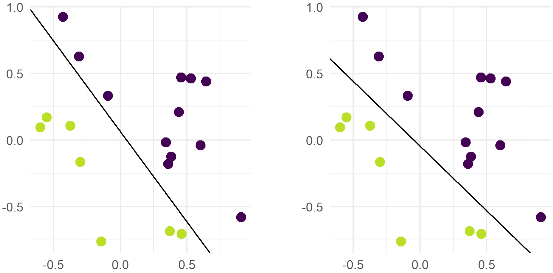
LINEAR SVM – METHOD SUMMARY

Optimization

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

Hyperparameters

Cost parameter C



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

LINEAR SVM – PRO’S & CON’S

Advantages

+ Often **sparse** solution (w.r.t. observations)
+ 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 (true for general regularized models).

Tuning

- Tuning of cost parameter *C* advisable ⇒ strong influence on resulting separating hyperplane
- Frequently, tuned on log-scale grid

Implementation

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

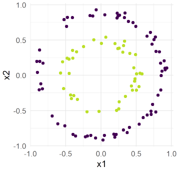
NONLINEAR SVM – METHOD SUMMARY

CLASSIFICATION REGRESSION NONPARAMETRIC BLACK-BOX

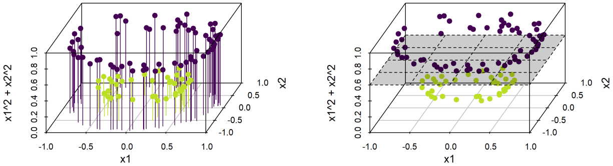
General idea

- Move **beyond linearity** by mapping data to transformed space where they are linearly separable
- **Kernel trick** (based on Mercer's theorem, existence of reproducing kernel Hilbert space):
  - Replace two-step operation feature map $\phi \rightsquigarrow$ inner product by **kernel** $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, 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
- Loss of interpretability through nonlinear feature map

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



Nonlinear problem in original space



Mapping to 3D space and subsequent linear separation – implicitly handled by kernel in nonlinear SVM

NONLINEAR SVM – METHOD SUMMARY

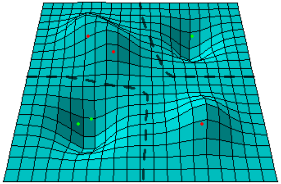
Dual problem **Kernelize** dual (soft-margin) SVM problem, replacing all inner products by kernels:

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

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 expressible 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
- Result: **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

Common kernels

- **Linear** kernel: dot product of given observations $\Rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x}^\top \tilde{\mathbf{x}}$ $\Rightarrow$ linear SVM
- **Polynomial** kernel of degree $d \in \mathbb{N}$: monomials (i.e., feature interactions) up to d-th order $\Rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \left(\mathbf{x}^\top \tilde{\mathbf{x}} + b\right)^d, \; b \geq 0$
- **Radial basis function (RBF)** kernel: infinite-dimensional feature space, 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`), with nonlinear kernel
- **Python:** `sklearn.svm.SVC` from package `scikit-learn` / package `libSVM`

K-NN – METHOD SUMMARY

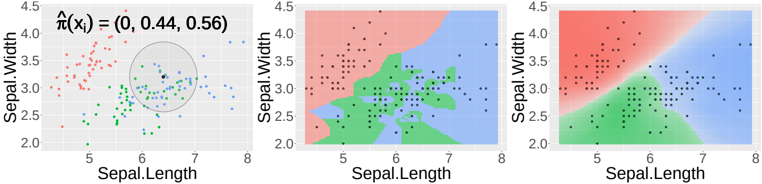
REGRESSION CLASSIFICATION NONPARAMETRIC WHITE-BOX

General idea

- Rationale: **similarity** in feature space $\rightsquigarrow$ similarity in target space w.r.t. certain **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**: $\hat{y} = 1 \Big/ \left(\sum_{i: \mathbf{x}^{(i)} \in N_k(\mathbf{x})} w_i\right) \sum_{i: \mathbf{x}^{(i)} \in N_k(\mathbf{x})} w_i y^{(i)}$
  - most frequent class for **classification**: $\hat{y} = \arg\max_{\ell \in \{1, \dots, g\}} \sum_{i: \mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$
- No distributional or functional **assumptions**
- **Nonparametric** behavior: parameters = training data; no compression of information
- Not immediately interpretable, but inspection of neighborhoods revealing

Hyperparameters

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



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

K-NN – PRO'S & CON'S

Advantages

- + **Easy** to explain and implement
- + 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 **nonlinear** decision boundaries
- + Easy to **tune**

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 more global model, i.e., 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 → $d(\mathbf{x}, \tilde{\mathbf{x}}) = \sum_j |x_j - \tilde{x}_j|$
  - $q = 2$: **Euclidean** distance → $d(\mathbf{x}, \tilde{\mathbf{x}}) = \sqrt{\sum_j (x_j - \tilde{x}_j)^2}$
- 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`

CART – METHOD SUMMARY

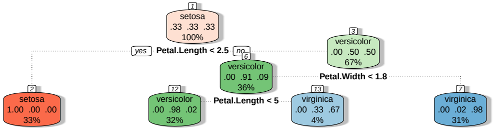
REGRESSION CLASSIFICATION NONPARAMETRIC WHITE-BOX FEATURE SELECTION

General idea

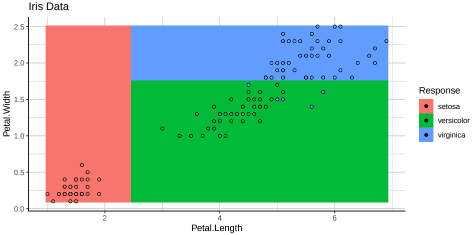
- Starting from root node containing all data, perform repeated **binary splits**, subsequently dividing input space into **rectangular partitions** Q_t
  - In each step, find **optimal split** (feature-threshold combination) → greedy search
  - Assign same response c_t to all observations in terminal 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



Corresponding prediction surface with axis-aligned boundaries

CART – METHOD SUMMARY

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** $\mathcal{R}(\mathcal{N}_t) = \sum\limits_{(\mathbf{x},y)\in\mathcal{N}_t} \sum\limits_{k=1}^{g} \hat{\pi}_k^{(\mathcal{N}_t)} \left(1 - \hat{\pi}_k^{(\mathcal{N}_t)}\right)$ → **Gini** impurity
    - **Bernoulli** loss $\mathcal{R}(\mathcal{N}_t) = \sum\limits_{(\mathbf{x},y)\in\mathcal{N}_t} - \sum\limits_{k=1}^{g} \hat{\pi}_k^{(\mathcal{N}_t)} \log \hat{\pi}_k^{(\mathcal{N}_t)}$ → **entropy** impurity
  - Regression: **quadratic** loss $\mathcal{R}(\mathcal{N}_t) = \sum\limits_{(\mathbf{x},y)\in\mathcal{N}_t} (y - c_t)^2$

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, ...

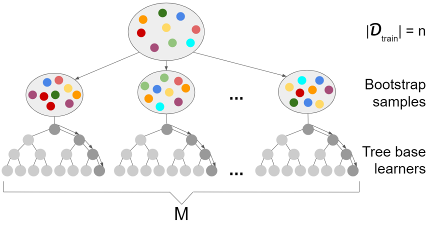
RANDOM FORESTS – METHOD SUMMARY

REGRESSION CLASSIFICATION NONPARAMETRIC BLACK-BOX FEATURE SELECTION

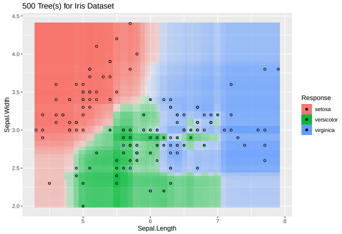
General idea

- 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
- **Predict** 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 – METHOD SUMMARY

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 individual trees' **interpretability** – at least, for large ensembles
- 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
⇒ 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` / `LearnerRegrRanger`, calling `ranger::ranger()`
- **Python:** `RandomForestClassifier` / `RandomForestRegressor` from package `scikit-learn`

GRADIENT BOOSTING – METHOD SUMMARY

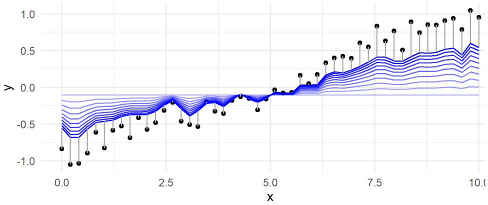
REGRESSION   CLASSIFICATION   (NON)PARAMETRIC   BLACK-BOX   FEATURE SELECTION

General idea

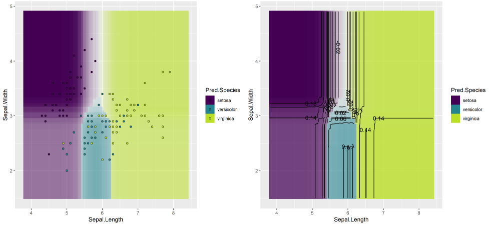
- Create **ensemble** in **sequential**, stage-wise manner
  - In each iteration, add new model component in risk-minimal fashion
  - Final model: weighted sum of base learners (frequently, **CART**)
- Fit each base learner to current **point-wise residuals**
  $\Rightarrow$ one boosting iteration $\widehat{=}$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

Empirical risk

- **Outer loss** used to compute pseudo-residuals – error of current model fit
  ⇒ arbitrary **differentiable** loss function
- **Inner loss** used to fit next base learner component to current pseudo-residuals
  ⇒ 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` / `LearnerRegrXgboost`, calling `xgboost::xgb.train()`
- **Python:** `GradientBoostingClassifier` / `GradientBoostingRegressor` from package `scikit-learn`, `XGBClassifier` / `XGBRegressor` from package `xgboost`

NEURAL NETWORKS – METHOD SUMMARY

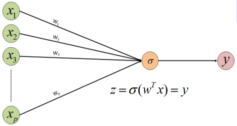
REGRESSION | CLASSIFICATION | (NON)PARAMETRIC | BLACK-BOX | FEATURE SELECTION

General idea

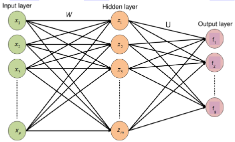
- Learn **composite function** through series of feature transformations, with components distributed over **neurons**, organized in **layers**
  - Basic neuron operation: 1) affine **transformation** with weights & bias term, 2) (nonlinear) **activation**
  - **Arbitrarily complex** combinations of fundamental building blocks
- Optimize 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 ⇒ gradients

Hypothesis space

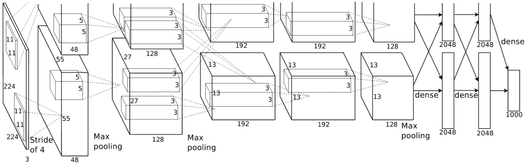
$$\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \tau \circ \phi \circ \sigma^{(h)} \circ \phi^{(h)} \circ \sigma^{(h-1)} \circ \phi^{(h-1)} \circ \ldots \circ \sigma^{(1)} \circ \phi^{(1)}(\mathbf{x}) \right\}$$



Single neuron



Feedforward network, 1 hidden layer



Convolutional network architecture

NEURAL NETWORKS – METHOD SUMMARY

Empirical risk Any **differentiable** loss function

Optimization

- Variety of different optimizers, mostly based on some form of **stochastic gradient descent**
- Backbone: gradient computation for arbitrary functions via **computational graphs**

NN types Large variety of architectures for different purposes

- **Feedforward NNs** / **multi-layer perceptrons (MLPs):** sequence of **fully-connected** layers
- **Convolutional NNs (CNNs):** sequence of feature map extractors with spatial awareness ⇒ images
- **Recurrent NNs (RNNs):** handling of sequential, variable-length information ⇒ times series, text, audio
- Unsupervised: **autoencoders**, **generative adversarial networks (GANs)**, . . .

Hyperparameters

- Regarding **architecture**
  - Lots of design choices ⇒ tuning problem of its own: **neural architecture search (NAS)**
  - E.g., network depth, layer types, activation functions, . . .
- Regarding **optimization & regularization**
  - Crucial due to **overparameterization** and strong **nonconvexity**
  - E.g., weight initialization, choice of optimizer, learning rate, batch size, number of epochs, . . .

NEURAL NETWORKS – PRO’S & CON’S

Advantages

- + Applicable to **complex, nonlinear** problems
- + Very **versatile** w.r.t. architectures
- + Suitable for **unstructured** data (e.g., images)
- + Strong **performance** if done right
- + Built-in **feature extraction**, obtained by intermediate representations
- + Easy handling of **high-dimensional** data
- + **Parallelizable** training

Disadvantages

- — Typically, high computational **cost**
- — High demand for **training data**
- — Strong tendency to **overfit**
- — Requiring lots of **tuning expertise**
- — **Black-box** model – hard to interpret or explain

Able to solve extremely complex tasks, but computationally expensive and hard to get right

NEURAL NETWORKS – PRACTICAL HINTS

Some options for regularization

- Control weight magnitude with **weight decay** (L2 regularization)
- Interrupt training when validation error starts to pick up ⇒ **early stopping**
- Use **dropout** to deactivate neurons at random, thus down-sizing network
- Expand training data and enforce invariances via **augmentation**
- . . .

Optimization tricks

- Accelerate training by incorporating **momentum**
- Control learning rate with **schedulers**, or keep it **adaptive**
- Use **batch normalization** for stability by keeping input distributions fixed throughout transformations
- . . .

Implementation

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