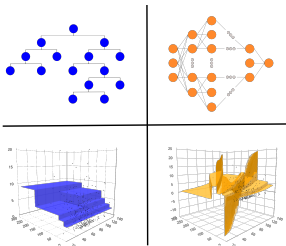
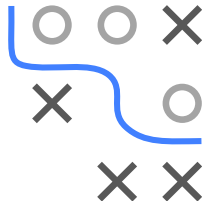


Important Learning Algorithms in ML



Learning goals

- General idea of important ML algorithms
- Overview of strengths and weaknesses

CONTENTS

- k -Nearest Neighbors (k -NN)
- Generalized Linear Models (GLM)
- Generalized Additive Models (GAM)
- Classification & Regression Trees (CART)
- Random Forests
- Gradient Boosting
- Linear Support Vector Machines (SVM)
- Nonlinear Support Vector Machines
- Neural Networks (NN)



K-NN – METHOD SUMMARY

REGRESSION

CLASSIFICATION

NONPARAMETRIC

WHITE-BOX

General idea

- **similarity** in feature space (w.r.t. certain **distance metric** $d(\mathbf{x}^{(i)}, \mathbf{x})$) \rightsquigarrow similarity in target space
- **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**: $\hat{y} = \frac{1}{\sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} w_i} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} w_i y^{(i)}$

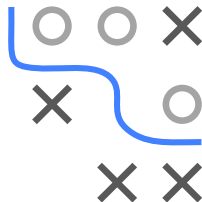
with $w_i = \frac{1}{d(\mathbf{x}^{(i)}, \mathbf{x})}$

→ optional: higher weights w_i for close neighbors

- most frequent class for **classification**: $\hat{y} = \arg \max_{\ell \in \{1, \dots, g\}} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$

⇒ Estimating posterior probabilities as $\hat{\pi}_\ell(\mathbf{x}^{(i)}) = \frac{1}{k} \sum_{i:\mathbf{x}^{(i)} \in N_k(\mathbf{x})} \mathbb{I}(y^{(i)} = \ell)$

- **Nonparametric** behavior: no compression of information
- Not immediately interpretable

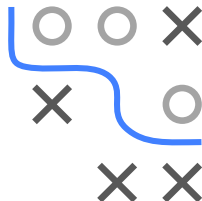


K-NN – IMPLEMENTATION & PRACTICAL HINTS

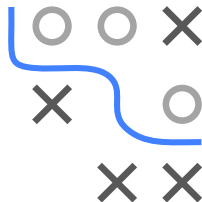
Preprocessing Features should be standardized or normalized

Implementation

- **R:** `mlr3` learners (calling `kknn::kknn()`)
 - **Classification:**
 - `LearnerClassifKKNN`
 - `fnn::knn()`
 - **Regression:**
 - `LearnerRegrKKNN`
 - `fnn::knn.reg()`
 - Nearest Neighbour Search in $\mathcal{O}(N \log N)$: `RANN::nn2()`



K-NN – IMPLEMENTATION & PRACTICAL HINTS



- **Python:** From package `sklearn.neighbors`
 - **Classification:**
 - `KNeighborsClassifier()`
 - `RadiusNeighborsClassifier()` as alternative if data not uniformly sampled
 - **Regression:**
 - `KNeighborsRegressor()`
 - `RadiusNeighborsRegressor()` as alternative if data not uniformly sampled

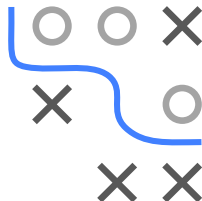
K-NN – PROS & CONS

Advantages

- + Algorithm **easy** to explain and implement
- + No distributional or functional **assumptions**
→ able to model data of **arbitrary complexity**
- + No **training** or **optimization** required
- + **local model** → **nonlinear** decision boundaries
- + Easy to **tune** (few hyperparameters)
→ number of neighbors k , distance metric
- + **Custom** distance metrics can often be easily designed to incorporate domain knowledge

Disadvantages

- Sensitivity w.r.t. **noisy** or **irrelevant** features and outliers due to dependency on distance measure
- Heavily affected by **curse of dimensionality**
- Bad performance when feature **scales** are not consistent with feature relevance
- Poor handling of data **imbalances** (worse for more global model, i.e., large k)



GENERALIZED LINEAR MODELS – METHOD SUMMARY

REGRESSION

CLASSIFICATION

PARAMETRIC

WHITE-BOX

FEATURE SELECTION

General idea Represent target as function of linear predictor $\theta^\top \mathbf{x}$ (weighted sum of features)

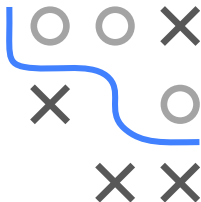
→ **Interpretation:** if feature x_j increases by 1 unit, the linear predictor changes by θ_j units

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

- **Linear Regression:** $\mathcal{Y} = \mathbb{R}$, ϕ identity
- **Logistic Regression:** $\mathcal{Y} = \{0, 1\}$, logistic sigmoid

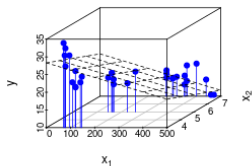
$$\phi(\theta^\top \mathbf{x}) = \frac{1}{1 + \exp(-\theta^\top \mathbf{x})} =: \pi(\mathbf{x} \mid \theta)$$

⇒ Decision rule: Linear hyperplane

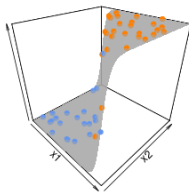
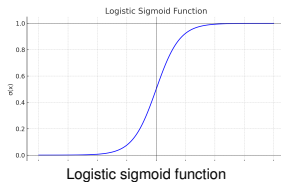


GENERALIZED LINEAR MODELS – METHOD SUMMARY

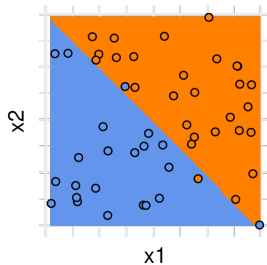
Loss functions



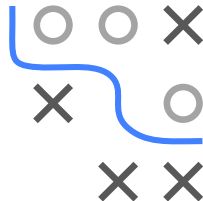
Linear regression hyperplane



Logistic function for bivariate input and loss-minimal θ



Corresponding separating hyperplane



GENERALIZED LINEAR MODELS – METHOD SUMMARY

- **Lin. Regr.:**

- Typically, based on **quadratic** loss (OLS estimation):

$$L(y, f) = (y - f)^2$$

- **Log. Regr.:** Based on **bernoulli / log / cross-entropy** loss

- Loss based on scores

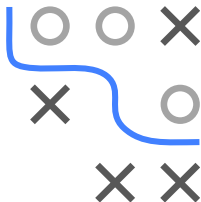
$$L(y, f) = \ln(1 + \exp(-y \cdot f)) \quad \text{for } y \in \{-1, +1\}$$

$$L(y, f) = -y \cdot f + \log(1 + \exp(f)) \quad \text{for } y \in \{0, 1\}$$

- Loss based on probabilities:

$$L(y, \pi) = \ln(1 + \exp(-y \cdot \log(\pi))) \quad \text{for } y \in \{-1, +1\}$$

$$L(y, \pi) = -y \log(\pi) - (1 - y) \log(1 - \pi) \quad \text{for } y \in \{0, 1\}$$



GENERALIZED LINEAR MODELS – METHOD SUMMARY

Optimization

- Minimization of the empirical risk
- For **OLS**: analytical solution $\hat{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$
- For other loss functions:
 - **Log. Regr.:** Convex problem, solvable via second-order optimization methods (e.g. BFGS)
 - **Else:** Numerical optimization



Multi-class extension of logistic regression

- Estimate **class-wise** scoring functions:

$$\Rightarrow \pi : \mathcal{X} \rightarrow [0, 1]^g, \pi(\mathbf{x}) = (\pi_1(\mathbf{x}), \dots, \pi_g(\mathbf{x})), \sum_{k=1}^g \pi_k(\mathbf{x}) = 1$$

- Achieved through **softmax** transformation:

$$\pi_k(\mathbf{x} | \theta) = \exp(\theta_k^\top \mathbf{x}) / \sum_{j=1}^g \exp(\theta_j^\top \mathbf{x})$$

- Multi-class log-loss: $L(y, \pi(\mathbf{x})) = - \sum_{k=1}^g \mathbb{I}_{\{y=k\}} \log(\pi_k(\mathbf{x}))$
- Predict class with maximum score (or use thresholding variant)

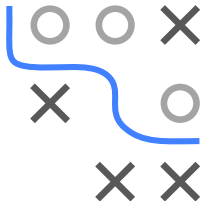
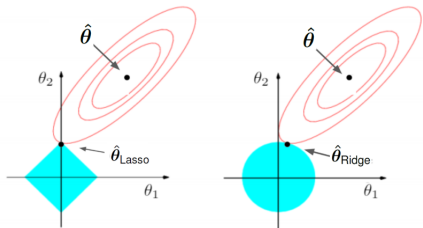
GENERALIZED LINEAR MODELS – REGULARIZATION

General idea

- Unregularized LM: risk of **overfitting** in high-dimensional space with only few observations
- **Goal**: avoidance of overfitting by adding **penalty term**

Regularized empirical risk

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



GENERALIZED LINEAR MODELS – REGULARIZATION

Optimization under regularization

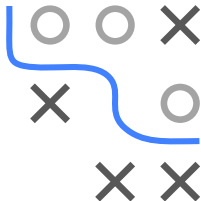
- **Ridge**: analytically with $\hat{\theta}_{\text{Ridge}} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$
- **LASSO**: numerically with, e.g., (sub-)gradient descent

Choice of regularization parameter

- Standard hyperparameter optimization problem
- E.g., choose λ with minimum mean cross-validated error

Ridge vs. LASSO

- **Ridge**
 - Global shrinkage \Rightarrow overall smaller but still dense θ
 - Applicable with large number of influential features, correlated variables' coefficients are shrunk by equal amount
- **LASSO**
 - Actual variable selection by shrinking coefficients to zero
 - Suitable for sparse problems, ineffective with correlated features (randomly selecting one)



GENERALIZED LINEAR MODELS – REGULARIZATION

- Neither overall better \Rightarrow **elastic net**
- Weighted combination of Ridge and LASSO
- Introducing additional penalization coefficient:

$$\mathcal{R}_{\text{reg}}(\theta) = \mathcal{R}_{\text{emp}}(\theta) + \lambda \cdot P_{\alpha}(\theta), \text{ with}$$

$$P_{\alpha}(\theta) = [\alpha \cdot \|\theta\|_1 + (1 - \alpha) \cdot \frac{1}{2} \cdot \|\theta\|_2^2]$$

Ridge performs better
for correlated features:

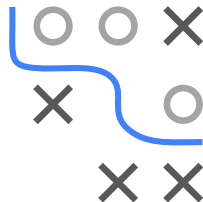
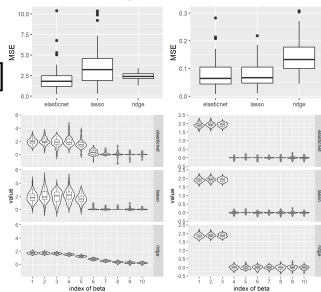
$$\beta = \underbrace{(2, \dots, 2)}_5, \underbrace{0, \dots, 0}_5$$

$$\text{cor}(\mathbf{X}_i, \mathbf{X}_j) = 0.8^{|i-j|}, \forall i, j$$

Lasso performs better
for uncorrelated features:

$$\beta = (2, 2, 2, \underbrace{0, \dots, 0}_7)$$

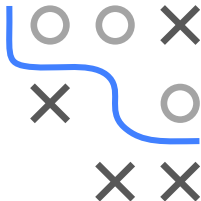
$$\text{cor}(\mathbf{X}_i, \mathbf{X}_j) = 0, \forall i \neq j$$



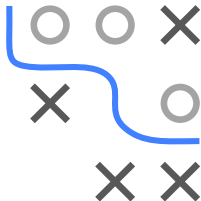
GENERALIZED LINEAR MODELS – IMPLEMENTATION

Implementation

- **R:**
 - **Unregularized:** `mlr3 learner LearnerRegrLM`, calling `stats::lm()` / `mlr3 learner LearnerClassifLogReg`, calling `stats::glm()`
 - **Regularized / ElasticNet:** `mlr3 learners LearnerClassifGlmnet / LearnerRegrGlmnet`, calling `glmnet::glmnet()`
 - For **large classification** data: `mlr3 learner LearnerClassifLiblinearR`, calling `LiblinearR::LiblinearR()` uses fast coordinate descent



GENERALIZED LINEAR MODELS – IMPLEMENTATION



- **Python:** From package `sklearn.linear_model`
 - **Unregularized:**
 - `LinearRegression()`
 - `LogisticRegression(penalty = None)`
 - **Regularized:**
 - *Linear regression:* `Lasso()`, `Ridge()`, `ElasticNet()`
 - *Logistic regression:* `LogisticRegression(penalty = {'l1', 'l2', 'elasticnet'})`
 - Package for advanced **statistical** models: `statsmodels.api`

GENERALIZED LINEAR MODELS – PROS & CONS

Advantages

- + **Simple and fast** implementation
- + **Analytical** solution for L2 loss
- + Applicable for any **dataset size**, as long as number of observations \gg number of features
- + Flexibility **beyond linearity** with polynomials, trigonometric transformations, interaction terms 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**: outliers, noise
- LM can **overfit** (e.g., many features and few observations)
- Feature **interactions** must be handcrafted
→ practically infeasible for higher orders



GENERALIZED ADDITIVE MODELS – METHOD SUMMARY

REGRESSION

CLASSIFICATION

(NON)PARAMETRIC

WHITE-BOX

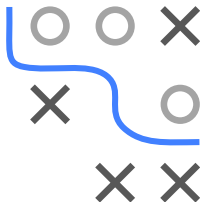
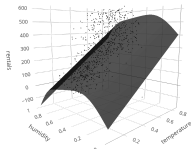
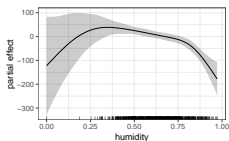
FEATURE SELECTION

General idea

- Same as GLM, but introduce **flexibility** through **nonlinear (smooth)** effects $f_j(x_j)$
- Typically, combination of linear & smooth effects
- Smooth effects also conceivable for feature interactions

Hypothesis space $\mathcal{H} = \left\{ f : \mathcal{X} \rightarrow \mathbb{R} \mid f(\mathbf{x}) = \phi \left(\theta_0 + \sum_{j=1}^p f_j(x_j) \right) \right\},$

suitable transformation $\phi(\cdot)$, intercept θ_0 , smooth functions $f_j(\cdot)$

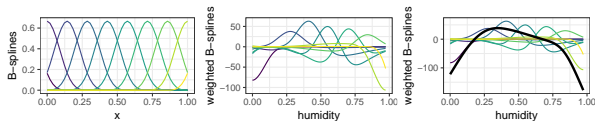


Prediction of bike rentals from smooth term of humidity (left: partial effect) and linear term of temperature (right: bivariate

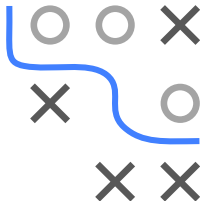
GENERALIZED ADDITIVE MODELS – METHOD SUMMARY

Smooth functions

- Non-/semi-/parametric approaches conceivable
- Frequently: express f_j as weighted sum of **basis functions** \rightsquigarrow model **linear** in weight coefficients again
 - Use fixed basis of functions b_1, \dots, b_K and estimate associated coefficients $\gamma_1, \dots, \gamma_K$
 $\rightsquigarrow f_j(x_j) = \sum_{k=1}^{K_j} \gamma_{j,k} b_k(x_j)$
 - Popular types of basis functions
 - Polynomial \rightsquigarrow smoothing/TP-/B-splines
 - Radial \rightsquigarrow **Kriging**
 - Trigonometric \rightsquigarrow **Fourier/wavelet** forms
- Alternatives: **local regression (LOESS)**, kernel-smoothing, ...



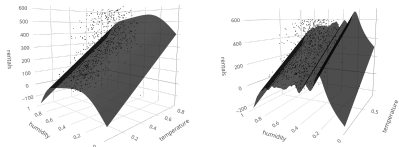
Left: B-spline basis with 9 basis functions. Middle: BFs weighted with coefficients estimated for humidity. Right: sum of weighted BFs in black (= partial effect).



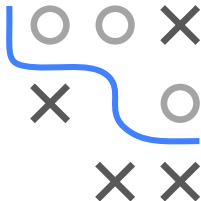
GENERALIZED ADDITIVE MODELS – METHOD SUMMARY

Regularization

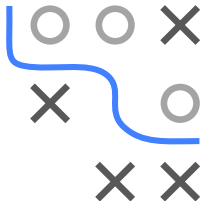
- Smooth functions possibly very flexible \rightsquigarrow regularization vital to prevent overfitting
- Control **smoothness**
 - **Basis-function approaches**: control number; impose penalty on coefficients (e.g., magnitude or differences between coefficients of neighboring components) & control associated hyperparameter
 - **Local smoothers**: control width of smoothing window (larger \rightsquigarrow smoother)



Prediction surfaces for bike rentals with 9 (left) and 500 (right) basis functions in smooth humidity term. Higher number of basis functions yields more local, less smooth model.



GENERALIZED ADDITIVE MODELS – METHOD SUMMARY

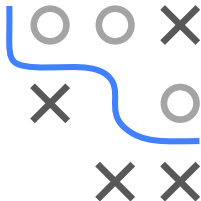


Loss functions Same as in GLM \rightsquigarrow essentially: use **negative log-likelihood**

Optimization

- **Coefficients** (of smooth + linear terms): penalized MLE, Bayesian inference
- **Smoothing hyperparameters**: typically, generalized cross-validation

GENERALIZED ADDITIVE MODELS – IMPLEMENTATION



Implementation

- **R:** `mlr3` learner `LearnerRegrGam`, calling `mgcv::gam()`
 - Smooth terms: `s(..., bs="<basis>")` or `te(...)` for multivariate (tensorproduct) effects
 - Link functions: `family={Gamma, Binomial, ...}`
- **Python:** `GLMGam` from package `statsmodels`; package `pygam`

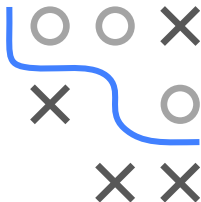
GENERALIZED ADDITIVE MODELS – PROS & CONS

Advantages

- + **Simple and fast**
- + Applicable for any **dataset size**, as long as number of observations \gg number of features
- + High **flexibility** via smooth effects
- + Easy to **combine** linear & nonlinear effects
- + Rather intuitive **interpretability** via feature effects
- + Statistical hypothesis **tests** for effects available

Disadvantages

- **Sensitivity** w.r.t. outliers and noisy data
- Feature **interactions** must be handcrafted
→ practically infeasible for higher orders
- Harder to **optimize** than GLM
- Additional **hyperparameters** (type of smooth functions, smoothness degree, ...)



CART – METHOD SUMMARY

REGRESSION

CLASSIFICATION

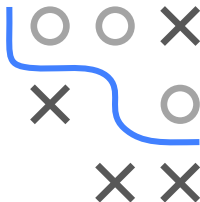
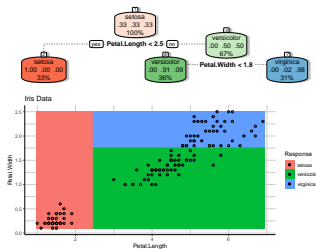
NONPARAMETRIC

WHITE-BOX

FEATURE SELECTION

General idea (CART – Classification and Regression Trees)

- Start at root node containing all data
- Perform repeated **axis-parallel binary splits** in feature space to obtain **rectangular partitions** at terminal nodes Q_1, \dots, Q_M
- Splits based on reduction of node **impurity**
→ empirical risk minimization (**ERM**)
- In each step:
 - Find **optimal split** (feature-threshold combination)
→ greedy search
 - Assign constant prediction c_m to all obs. in Q_m
→ Regression: c_m is average of y
→ Classif.: c_m is majority class (or class proportions)
 - Stop when a pre-defined criterion is reached
→ See **Complexity control**

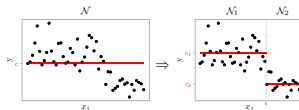


CART – METHOD SUMMARY

Hypothesis space $\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \sum_{m=1}^M c_m \mathbb{I}(\mathbf{x} \in Q_m) \right\}$

Empirical risk

- Splitting **feature** x_j at **split point** t divides a parent node N_p into two child nodes:

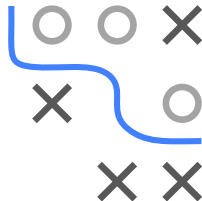


$$N_l = \{(\mathbf{x}, y) \in N_p : x_j \leq t\} \text{ and } N_r = \{(\mathbf{x}, y) \in N_p : x_j > t\}$$

- Compute empirical risks in child nodes and minimize their sum to find best split (impurity reduction):

$$\arg \min_{i,t} \mathcal{R}(N_p, j, t) = \arg \min_{i,t} \mathcal{R}(N_l) + \mathcal{R}(N_r) \quad (1)$$

Note: If \mathcal{R} is the average instead of the sum of loss functions, we need to

$$\text{reweight: } \frac{|N_{pt}|}{|N_p|} \mathcal{R}(N_{pt})$$


CART – METHOD SUMMARY

- In general, compatible with arbitrary losses – typical choices:

- g -way classification:

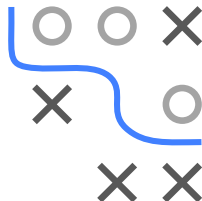
Brier score \rightarrow Gini impurity	Bernoulli loss \rightarrow entropy impurity
$\mathcal{R}(N_p) = \sum_{(\mathbf{x}, y) \in N_p} \sum_{k=1}^g \hat{\pi}_k^{(N_p)} (1 - \hat{\pi}_k^{(N_p)})$	$\mathcal{R}(N_p) = - \sum_{(\mathbf{x}, y) \in N_p} \sum_{k=1}^g \hat{\pi}_k^{(N_p)} \log \hat{\pi}_k^{(N_p)}$

- Regression (**quadratic** loss): $\mathcal{R}(N_p) = \sum_{(\mathbf{x}, y) \in N_p} (y - c)^2$ with

$$c = \frac{1}{|N_p|} \sum_{(\mathbf{x}, y) \in N_p} y$$

Optimization

- **Exhaustive** search over all split candidates, choice of risk-minimal split
- In practice: reduce number of split candidates (e.g., using quantiles instead of all observed values)



CART – IMPLEMENTATION & PRACTICAL HINTS

Hyperparameters and complexity control

- Unless interrupted, splitting continues until we have pure leaf nodes (costly + overfitting)
- Hyperparameters: Complexity (i.e., number of terminal nodes) controlled via tree depth, minimum number of observations per node, maximum number of leaves, minimum risk reduction per split, ...
- Limit tree growth / complexity via
 - **Early stopping:** stop growth prematurely
→ hard to determine good stopping point before actually trying all combinations
 - **Pruning:** grow deep trees and cut back in risk-optimal manner afterwards



CART – IMPLEMENTATION & PRACTICAL HINTS

Implementations

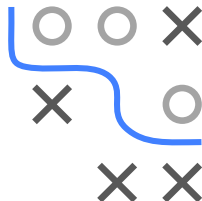
- **R:**

- **CART:** `mlr3` learners `LearnerClassifRpart / LearnerRegrRpart`, calling `rpart::rpart()`
- **Conditional inference trees:** `partykit::ctree()`
mitigates overfitting by controlling tree size via p-value-based splitting
- **Model-based recursive partitioning:** `partykit::mob()`
fits a linear model within each terminal node of the decision tree
- **Rule-based models:** `Cubist::cubist()` for regression and `C50::C5.0()` for classification; more flexible frameworks for fitting various types of models (e.g., GLMs) within a tree's terminal nodes

- **Python:** `DecisionTreeClassifier / DecisionTreeRegressor`
from package `scikit-learn`



CART – PROS & CONS



Dual purpose of CART

- **Exploration purpose** to obtain interpretable decision rules (here: performance/tuning is secondary)
- **Prediction model**: CART as base learner in **ensembles** (bagging, random forest, boosting) can improve stability and performance (if tuned properly), but becomes less interpretable

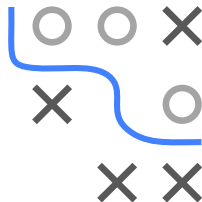
CART – PROS & CONS

Advantages

- + **Easy** to understand & visualize (**interpretable**)
- + Built-in **feature selection**
→ e.g., when features are not used for splitting
- + Applicable to **categorical** features
→ e.g., 2^m possible binary splits for m categories
→ trick for regr. with L2-loss and binary classif.: categories can be sorted $\Rightarrow m - 1$ binary splits
- + Handling of **missings** possible via surrogate splits
- + Models **interactions**,
- + **Fast** well scalable
- + High **flexibility** with custom split criteria or leaf-node prediction rules

Disadvantages

- Rather **poor generalization**
- High **variance/instability**: model can change a lot when training data is minimally changed
- Can **overfit** if tree is grown too deep
- Not well-suited to model **linear** relationships
- **Bias** toward features with many unique values or categories



RANDOM FORESTS – METHOD SUMMARY

REGRESSION

CLASSIFICATION

NONPARAMETRIC

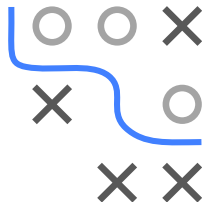
BLACK-BOX

FEATURE SELECTION

General idea

- **Bagging ensemble** of M tree **base learners** fitted on **bootstrap** data samples
 - ⇒ Reduce **variance** by ensembling while slightly increasing **bias** by bootstrapping
 - Use unstable, **high-variance** base learners by letting trees grow to full size
 - Promoting **decorrelation** by random subset of candidate features for each split
- **Predict** via averaging (regression) or majority vote (classification) of base learners

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



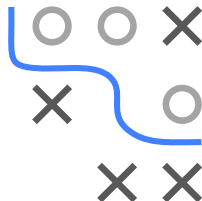
RANDOM FORESTS – METHOD SUMMARY

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

Hyperparameters

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



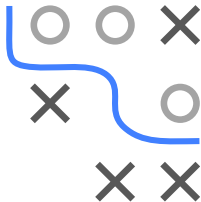
RANDOM FORESTS – IMPLEMENTATION & PRACTICAL HINTS

Extremely Randomized Trees

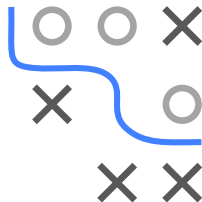
- Variance of trees can be further increased by **randomizing split points** instead of using the optimal one
- Alternatively consider k random splits and pick the best one according to impurity

Tuning

- **Ensemble size** should not be tuned as it only decreases variance
—→ choose sufficiently large ensemble
- While default values for **number of split points** is often good, tuning it can still improve performance
- Tuning the **minimum samples in leafs** and **minimum samples for splitting** can be beneficial but no huge performance increases are to be expected



RANDOM FORESTS – IMPLEMENTATION & PRACTICAL HINTS



Implementation

- **R:** `mlr3` learners `LearnerClassifRanger` / `LearnerRegrRanger`, calling `ranger::ranger()` as a highly efficient and flexible implementation
- **Python:** `RandomForestClassifier` / `RandomForestRegressor` from package `scikit-learn`

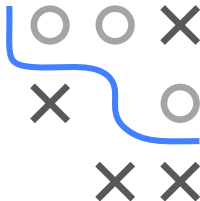
RANDOM FORESTS – PROS & CONS

Advantages

- + Retains most of **trees'** advantages (e.g., feature selection, feature interactions)
- + Fairly **good predictor**: mitigating base learners' variance through bagging
- + Quite **robust** w.r.t. small changes in data
- + Good with **high-dimensional** data, even in presence of noisy features
- + Easy to **parallelize**
- + Robust to its hyperparameter configuration
- + Intuitive measures of **feature importance**

Disadvantages

- Loss of individual trees' **interpretability**
- Can be suboptimal for **regression** when extrapolation is needed
- **Bias** toward selecting features with many categories (same as CART)
- Rather large model size and slow inference time for large ensembles
- Typically inferior in **performance** to tuned gradient tree boosting.



GRADIENT BOOSTING – METHOD SUMMARY

REGRESSION

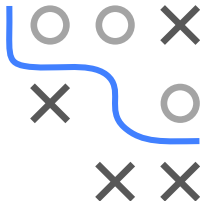
CLASSIFICATION

BLACK-BOX

FEATURE SELECTION

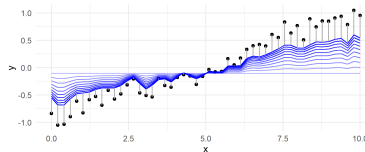
General idea

- **Sequential ensemble** of M **base learners** by greedy forward stagewise additive modeling
 - In each iteration a base learner is fitted to current **pseudo residuals** \Rightarrow one boosting iteration is one approximate **gradient step in function space**
 - Base learners are typically **trees**, **linear regressions** or **splines**
- **Predict** via (weighted) sum of base learners

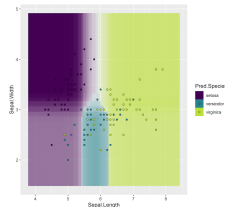


GRADIENT BOOSTING – METHOD SUMMARY

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



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)



Empirical risk

- In general, compatible with any **differentiable** loss
- Base learner in iteration m is fitted on **Pseudo residuals**:

$$\tilde{r}^{(i)} = -\frac{\partial L(y^{(i)}, f(\mathbf{x}^{(i)}))}{\partial f(\mathbf{x}^{(i)})} \text{ by minimizing the L2-loss: } \sum_{i=1}^n (\tilde{r}^{(i)} - b(\mathbf{x}^{(i)}, \theta))^2$$

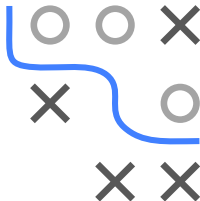
GRADIENT BOOSTING – METHOD SUMMARY

Optimization

- Same optimization procedure as base learner, while keeping the current ensemble $fmdh$ fixed
 \Rightarrow Efficient and generally applicable since *inner* loss is always L2
- βm is found via **line search** or fixed to a **small constant value** and combined with the leaf values ctm for tree base learners:
 $ctmt = \beta m \cdot ctm$

Hyperparameters

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



GRADIENT BOOSTING – PRACTICAL HINTS

- ## Scalable Gradient Boosting

Explainable / Componentwise Gradient Boosting

- Base learners of **simple linear regression** models or **splines**, selecting a single feature in each iteration
- Allows **feature selection** and creates an **interpretable** model since uni- and bivariate effects can be visualized directly.
- Feature interactions can be learned via ranking techniques (e.g., GA²M FAST)

Tuning

- Use **early-stopping** to determine ensemble size
- Various **regularization parameters**, e.g., L1/L2, number of leaves, ... that need to be carefully tuned
- Tune learning rate and base learner complexity hyperparameters on **log-scale**

- + Retains of most of **base learners'** advantages
- + Very **good predictor** due to aggressive loss minimization, typically only outperformed by heterogenous **stacking ensembles**
- + High **flexibility** via custom loss functions and choice of base learner
- + Highly efficient implementations exist (`lightgbm` / `xgboost`) that work well on large (distributed) data sets
- + Componentwise boosting: Good combination of (a) high performance (b) interpretable model and (c) feature selection

- Loss of base learners' potential **interpretability**
- **Many hyperparameters** to be carefully tuned
- Hard to **parallelize** (\leadsto solved by efficient implementation)

LINEAR SVM – METHOD SUMMARY

CLASSIFICATION

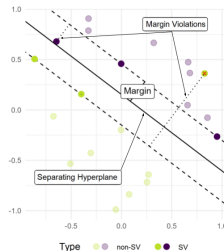
REGRESSION

PARAMETRIC

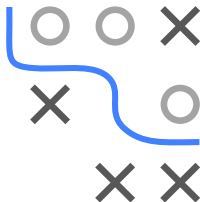
WHITE-BOX

highlightGeneral idea (Soft-margin SVM)

- Find linear decision boundary (**separating hyperplane**) that
 - maximizes distance (**margin γ**) to closest points (**support vectors, SVs**) on each side of decision boundary
 - while minimizing margin violations (points either on **wrong side of hyperplane** or **between dashed margin line and hyperplane**)
- 3 types of training points
 - **non-SVs** with no impact on decision boundary
 - **SVs that are margin violators** and affect decision boundary
 - **SVs located exactly on dashed margin lines** and affect decision boundary



Soft-margin SVM with margin violations



LINEAR SVM – METHOD SUMMARY

Hypothesis space (primal) $\mathcal{H} = \{f(\mathbf{x}) : f(\mathbf{x}) = \theta^\top \mathbf{x} + \theta_0\}$

Empirical risk Soft-margin

SVM as L2-regularized ERM:

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

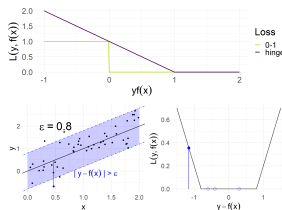
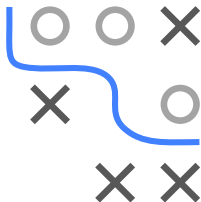
- $\|\theta\| = 1/\gamma$ ($\hat{=}$ maximizing margin)
- $C > 0$: penalization for margin violations
- Loss aims at minimizing margin violations

→ Classif. (**hinge** loss):

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

→ Regr. (ϵ -**insensitive** loss):

$$L(y, f) = \max(|y - f| - \epsilon, 0)$$



LINEAR SVM – METHOD SUMMARY

Dual problem SVMs as a constraint optimization (primal) problem (maximize margin s.t. constraints on obs. to limit margin violations) can be formulated as a Lagrangian dual problem with Lagrange multipliers $\alpha_i \geq 0$:

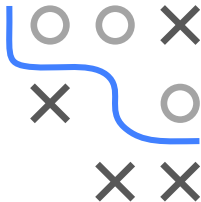
$$\max_{\alpha \in \mathbb{R}^n} \Leftrightarrow \text{ s.t. } 0 \leq \alpha_i \leq C \quad \forall i \in \{1, \dots, n\} \text{ and } \sum_{i=1}^n \alpha_i y^{(i)} = 0$$

Solution Non-SVs have $\alpha_i = 0$ as they do not affect the hyperplane

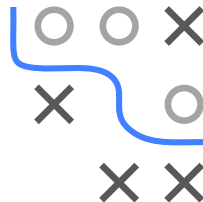
$$f(\mathbf{x}) = \sum_{i=1}^n \alpha_i y^{(i)} \langle \mathbf{x}^{(i)}, \mathbf{x} \rangle + \theta_0$$

Optimization

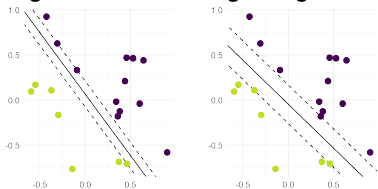
- Typically, tackling **dual** problem (though feasible in corresponding primal) via **quadratic programming**
- Popular: **sequential minimal optimization** \Rightarrow iterative algorithm based on breaking down objective into bivariate quadratic problems with analytical solutions



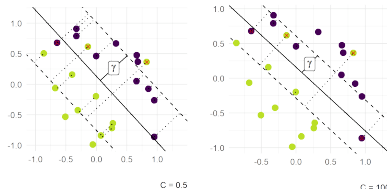
LINEAR SVM – METHOD SUMMARY



Hyperparameters Cost parameter C to control maximization of the margin vs. minimizing margin violations



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

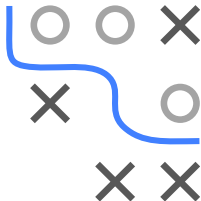
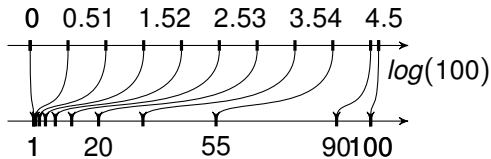


Soft-margin SVM: large margin and few margin violations on the right (best trade-off)

Preprocessing Features should be scaled before applying SVMs
(applies generally to regularized models)

Tuning

- Tuning of cost parameter C advisable
⇒ strong influence on resulting hyperplane
- C it is often tuned on a log-scale grid for optimal and space-filling search space



LINEAR SVM – IMPLEMENTATION

Implementation

- **R:** `mlr3` learners `LearnerClassifSVM` / `LearnerRegrSVM`, calling `e1071::svm()` with linear kernel (`libSVM` interface). Further implementations in `mlr3extralearners` based on
 - `kernlab::ksvm()` allowing custom kernels
 - `LiblinearR::LiblinearR()` for a fast implementation 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**
 - No need for explicit construction of feature maps
 - Replace inner product of feature map $\phi : \mathcal{X} \rightarrow \Phi$ by **kernel**:
 $\langle \phi \mathbf{x}, \phi \mathbf{x}' \rangle = k(\mathbf{x}, \mathbf{x}')$

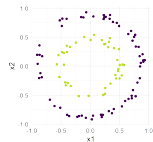


Hypothesis space

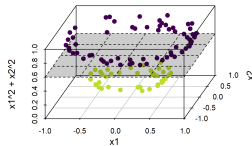
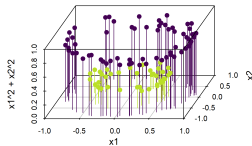
$$\mathcal{H} = \{f(\mathbf{x}) : f(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^\top \phi \mathbf{x} + \theta_0)\} \text{ (primal)}$$

$$\mathcal{H} = \left\{f(\mathbf{x}) : f(\mathbf{x}) = \text{sign}\left(\sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0\right) \mid \alpha_i \geq 0, \sum_{i=1}^n \alpha_i y^{(i)} = 0\right\} \text{ (dual)}$$

centering

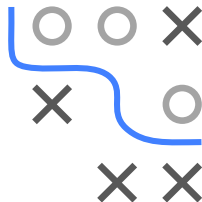


Nonlinear problem in original space



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:

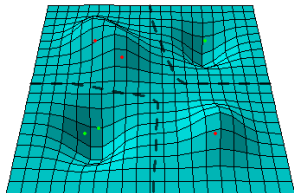
$$\max_{\alpha} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}), \quad \text{s.t.} \quad 0 \leq \alpha_i \leq C, \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0.$$

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

NONLINEAR SVM – METHOD SUMMARY

Interpretation as basis function approach

- **Representer theorem:** solution of dual soft-margin SVM problem is $\theta = \sum_{j=1}^n \beta_j \phi(\mathbf{x}^{(j)})$
- Sparse, weighted sum of **basis functions**
 $\rightarrow \beta_j = 0$ for non-SVs
- Result: **local** model with smoothness depending on kernel



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



NONLINEAR SVM – IMPLEMENTATION & PRACTICAL HINTS

Common kernels

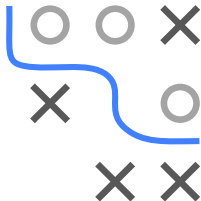
- **Linear** kernel: dot product of given observations $\Rightarrow k_{xxt} = \mathbf{x}^\top \tilde{\mathbf{x}} \Rightarrow$ linear SVM
- **Polynomial** kernel of degree $d \in \mathbb{N}$: monomials (i.e., feature interactions) up to d -th order $\Rightarrow k_{xxt} = (\mathbf{x}^\top \tilde{\mathbf{x}} + b)^d, b \geq 0$
- **Radial basis function (RBF)** kernel: infinite-dimensional feature space, allowing for perfect separation of all finite datasets $\Rightarrow k_{xxt} = \exp(-\gamma \|\mathbf{x} - \tilde{\mathbf{x}}\|_2^2)$ 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()` with nonlinear kernel (`libSVM` interface), `kernlab::ksvm()` allowing custom kernels
- **Python:** `sklearn.svm.SVC` from package `scikit-learn` / package `libSVM`



SVM – PRO'S & CON'S

Advantages

- + Often **sparse** solution (w.r.t. observations)
- + Robust against overfitting (**regularized**); especially in high-dimensional space
- + **Stable** solutions (w.r.t. changes in train data)
 - Non-SV do not affect decision boundary
- + Convex optimization problem
 - local minimum $\hat{=}$ global minimum

Disadvantages

- **Long** training times $\rightarrow O(n^2p + n^3)$
- Confined to **linear model**
- Restricted to **continuous features**
- Optimization can also fail or get stuck



SVM – PRO'S & CON'S

Advantages (nonlinear SVM)

- + Can learn **nonlinear decision boundaries**
- + **Very flexible** due to custom kernels
 - RBF kernel yields local model
 - kernel for time series, strings etc.

Disadvantages (nonlinear SVM)

- Poor **interpretability** due to complex kernel
- **Not easy tunable** as it is highly important to choose the right kernel (which also introduces further hyperparameters)



NEURAL NETWORKS – METHOD SUMMARY

REGRESSION

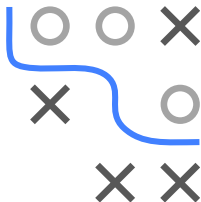
CLASSIFICATION

(NON)PARAMETRIC

BLACK-BOX

General idea

- Learn **composite function** through series of nonlinear feature transformations, represented as **neurons**, organized hierarchically in **layers**
 - Basic neuron operation: 1) affine **transformation** ϕ (weighted sum of inputs), 2) nonlinear **activation** σ
 - Combinations of simple building blocks to create a complex model
- Optimize via **mini-batch stochastic gradient descent (SGD)**
variants:
 - Gradient of each weight can be inferred from the **computational graph** of the network
→ **Automatic Differentiation** (AutoDiff)
 - Algorithm to compute weight updates based on the loss is called **Backpropagation**



Hypothesis space $\mathcal{H} =$

$$\{f(\mathbf{x}) : f(\mathbf{x}) = \tau \circ \phi \circ \sigma^{(h)} \circ \phi^{(h)} \circ \sigma^{(h-1)} \circ \phi^{(h-1)} \circ \dots \circ \sigma^{(1)} \circ \phi^{(1)}(\mathbf{x})\}$$

NEURAL NETWORKS – IMPLEMENTATION & PRACTICAL HINTS

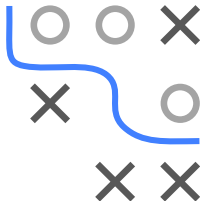
General hints

- Instead of NAS, use a standard architecture and tune training hyperparameters
- Training pipeline (data-augmentation, training schedules, ...) is more crucial than the specific architecture
- While NNets are state-of-the-art for **computer vision (CV)** and **natural language processing (NLP)**, we recommend not to use them for tabular data because alternatives perform better
- Computational efforts for training (and inference) can be very high, requiring specific hardware.
→ Using a service (esp. for foundation models) can be more cost efficient

Implementation

- **R:** Use python libraries (below) via `reticulate`, but not really recommended except for toy applications.
- **Python libraries:**

- `keras` for simple high level API



NEURAL NETWORKS – PROS & CONS

Advantages

- + Applicable to **complex, nonlinear** problems
- + Very **versatile** w.r.t. architectures
- + State-of-the-art for CV and NLP
- + 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

