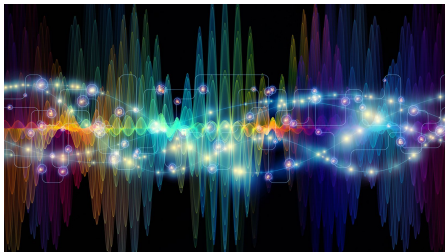


Important Learners in ML



Learning goals

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

CONTENTS

- 1 k -Nearest Neighbors (k -NN)
- 2 Generalized Linear Models (GLM)
- 3 Generalized Additive Models (GAM)
- 4 Classification & Regression Trees (CART)
- 5 Random Forests
- 6 Gradient Boosting
- 7 Linear Support Vector Machines (SVM)
- 8 Nonlinear Support Vector Machines
- 9 Gaussian Processes (GP)
- 10 Neural Networks (NN)

K-NN – METHOD SUMMARY

REGRESSION

CLASSIFICATION

NONPARAMETRIC

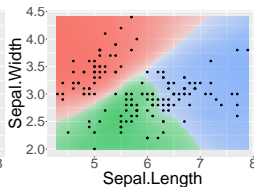
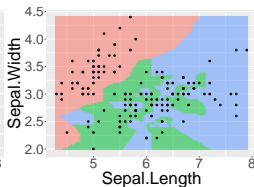
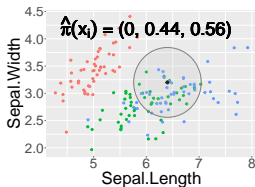
WHITE-BOX

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: parameters = training data; no compression of information
- Not immediately interpretable, but inspection of neighborhoods can be revealing

K-NN – METHOD SUMMARY

Hyperparameters Neighborhood **size** k (locality), **distance** metric (next page)

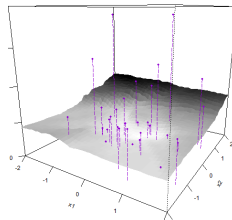
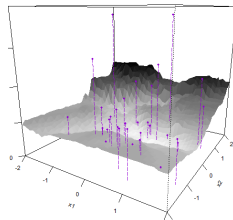
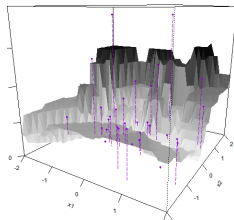


Classification

Left: Neighborhood for exemplary observation in iris, $k = 50$

Middle: Prediction surface for $k = 1$

Right: Prediction surface for $k = 50$



Regression

Left: Prediction surface for $k = 3$

Middle: Prediction surface for $k = 7$

Right: Prediction surface for $k = 15$

- Small $k \Rightarrow$ very local, "wiggly" decision boundaries
- Large $k \Rightarrow$ rather global, smooth decision boundaries

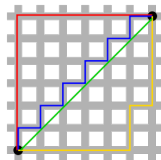
K-NN – METHOD SUMMARY

Popular distance metrics

- Numerical feature space:

⇒ 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 $\rightarrow d(\mathbf{x}, \tilde{\mathbf{x}}) = \sqrt{\sum_j (x_j - \tilde{x}_j)^2}$
- Visualization: Manhattan (red, blue, yellow) vs. Euclidean (green)



- Mixed feature space:

- **Gower distance** can handle numerical and categorical features, and missing data:

- numerical: $d(x_i, x_j) = \frac{|x_i - x_j|}{\max(x) - \min(x)}$
- categorical: $d(x_i, x_j) = \begin{cases} 1, & \text{if } x_i \neq x_j \\ 0, & \text{if } x_i = x_j \end{cases}$
- Gower distance as average over individual scores

- Optional **weighting** to account for beliefs about varying feature importance

Figure Source: https://es.m.wikipedia.org/wiki/Archivo:Manhattan_distance.svg

K-NN – IMPLEMENTATION & PRACTICAL HINTS

Preprocessing Features should be standardized or normalized

Implementation

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

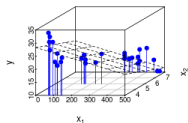
FEATURE SELECTION

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

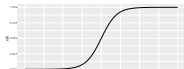
→ **Interpretation:** if feature x_j increases by 1 unit, the linear predictor changes by θ_j units

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.,

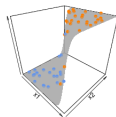
- **Linear Regression:** $\mathcal{Y} = \mathbb{R}$, ϕ identity
- **Logistic Regression:** $\mathcal{Y} = \{0, 1\}$, logistic sigmoid $\phi(\theta^\top \mathbf{x}) = \frac{1}{1 + \exp(-\theta^\top \mathbf{x})} =: \pi(\mathbf{x} \mid \theta)$
⇒ Decision rule: Linear hyperplane



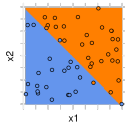
Linear regression hyperplane



Logistic sigmoid function



Logistic function for bivariate input and loss-minimal θ



Corresponding separating hyperplane

GENERALIZED LINEAR MODELS – METHOD SUMMARY

Loss functions

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

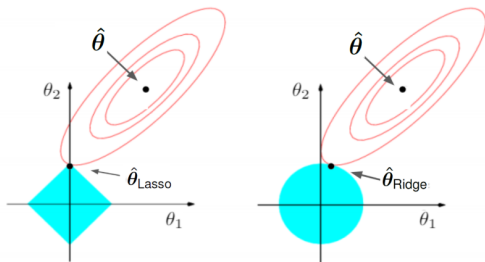
- Empirical risk function **plus complexity penalty** $J(\theta)$, controlled by shrinkage parameter $\lambda > 0$:
 $\mathcal{R}_{\text{reg}}(\theta) := \mathcal{R}_{\text{emp}}(\theta) + \lambda \cdot J(\theta)$
- **Ridge** regression: L2 penalty $J(\theta) = \|\theta\|_2^2$
- **LASSO** regression: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

Optimization under regularization

- **Ridge**: analytically with $\hat{\theta}_{\text{Ridge}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$
- **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



GENERALIZED LINEAR MODELS – REGULARIZATION

Ridge vs. LASSO

● Ridge

- Global shrinkage \Rightarrow overall smaller but still dense θ
- Applicable with large number of influential features, handling correlated variables by shrinking their coefficients by equal amount

● 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**

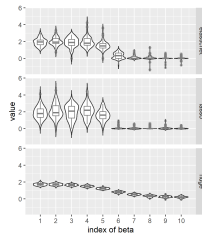
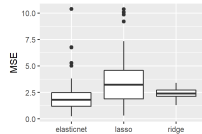
- Weighted combination of Ridge and LASSO
- Introducing additional penalization coefficient:

$$\mathcal{R}_{\text{reg}}(\theta) = \mathcal{R}_{\text{emp}}(\theta) + \lambda \cdot P_{\alpha}(\theta), \text{ with}$$
$$P_{\alpha}(\theta) = [\alpha \cdot \|\theta\|_1 + (1 - \alpha) \cdot \frac{1}{2} \cdot \|\theta\|_2^2]$$

Ridge performs better for correlated features:

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

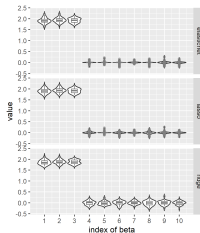
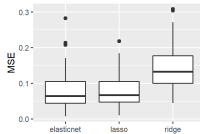
$$\text{cor}(\mathbf{X}_i, \mathbf{X}_j) = 0.8^{|i-j|}, \forall i, j$$



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 `LearnerClassifLiblineaR`, calling `LiblineaR::LiblineaR()` uses fast coordinate descent
- **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** w.r.t. outliers and noisy data (especially with L2 loss)
- Also a 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

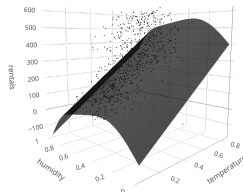
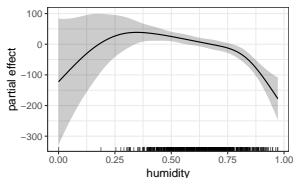
WHITE-BOX

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 $\mathcal{H} = \left\{ f : \mathcal{X} \rightarrow \mathbb{R} \mid f(\mathbf{x}) = \phi \left(\theta_0 + \sum_{j=1}^p f_j(x_j) \right) \right\}$, with suitable transformation $\phi(\cdot)$,
intercept term θ_0 , and smooth functions $f_j(\cdot)$

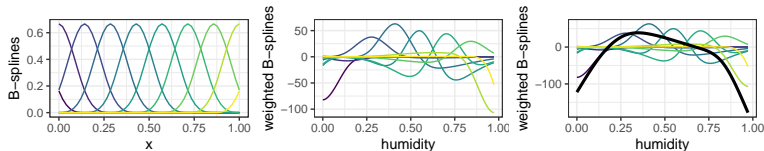


Prediction of bike rentals from smooth term of humidity (left: partial effect) and linear term of temperature (right: bivariate prediction).

GENERALIZED ADDITIVE MODELS – METHOD SUMMARY

Smooth functions

- Nonparametric/semiparametric/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)**, other kernel-smoothing approaches, ...

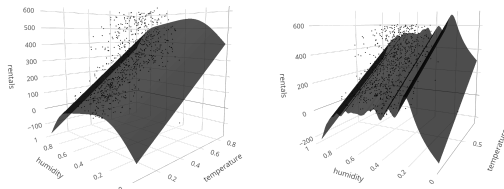


Left: B-spline basis with 9 basis functions. Middle: BFs weighted with coefficients estimated for `humidity`. Right: sum of weighted BFs in black (= partial effect).

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.

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`

Advantages

- + **Simple and fast** implementation
- + 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
- + Intuitive **interpretability** via feature effects (though not quite as straightforward as in GLM)
- + 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

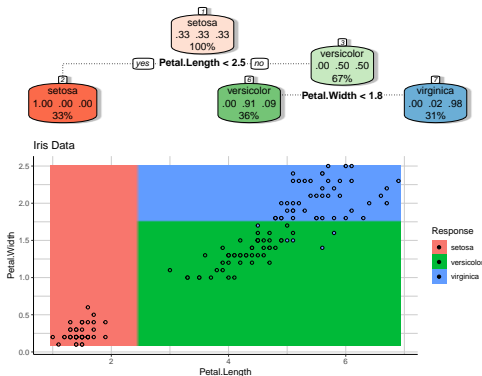
WHITE-BOX

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**

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

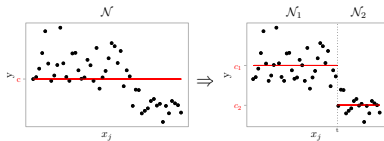


CART – METHOD SUMMARY

Empirical risk

- Splitting **feature** x_j **at split point** t divides a parent node \mathcal{N} into two child nodes:

$$\mathcal{N}_1 = \{(\mathbf{x}, y) \in \mathcal{N} : x_j \leq t\} \text{ and } \mathcal{N}_2 = \{(\mathbf{x}, y) \in \mathcal{N} : x_j > t\}$$



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

$$\arg \min_{j,t} \mathcal{R}(\mathcal{N}, j, t) = \arg \min_{j,t} \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2)$$

Note: If \mathcal{R} is the average instead of the sum of loss functions, we need to reweight: $\frac{|\mathcal{N}_t|}{|\mathcal{N}|} \mathcal{R}(\mathcal{N}_t)$

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

Brier score \rightarrow Gini impurity	Bernoulli loss \rightarrow entropy impurity
$\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x}, y) \in \mathcal{N}} \sum_{k=1}^g \hat{\pi}_k^{(\mathcal{N})} (1 - \hat{\pi}_k^{(\mathcal{N})})$	$\mathcal{R}(\mathcal{N}) = - \sum_{(\mathbf{x}, y) \in \mathcal{N}} \sum_{k=1}^g \hat{\pi}_k^{(\mathcal{N})} \log \hat{\pi}_k^{(\mathcal{N})}$
<ul style="list-style-type: none">Regression (quadratic loss): $\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x}, y) \in \mathcal{N}} (y - c)^2$ with $c = \frac{1}{ \mathcal{N} } \sum_{(\mathbf{x}, y) \in \mathcal{N}} y$	

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

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

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**, even of higher order
- + **Fast** computation and good scalability
- + 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

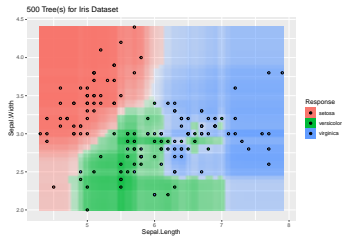
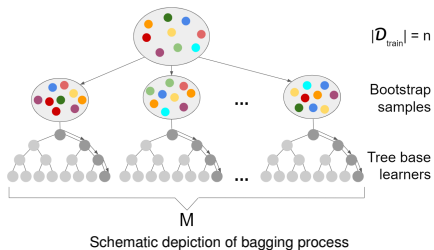
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FEATURE SELECTION

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



Prediction surface for iris data with 500-tree ensemble

RANDOM FORESTS – METHOD SUMMARY

Empirical risk & Optimization Just like tree base learners

Out-of-bag (OOB) error

- Ensemble prediction for obs. outside individual trees' bootstrap training sample \Rightarrow unseen test sample
- Use resulting loss as unbiased estimate of **generalization error**
- Mainly useful for tuning and less for model comparison as we usually compare all models uniformly by CV

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
 \Rightarrow 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

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

(NON)PARAMETRIC

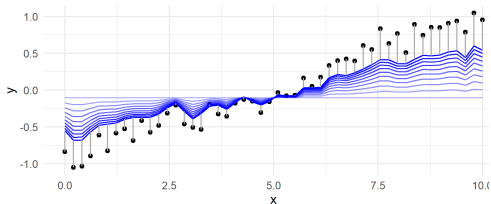
BLACK-BOX

FEATURE SELECTION

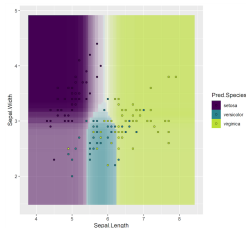
General idea

- **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

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)

GRADIENT BOOSTING – METHOD SUMMARY

Empirical risk

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

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

Optimization

- Same optimization procedure as base learner, while keeping the current ensemble $\hat{f}^{[m-1]}$ fixed
⇒ Efficient and generally applicable since *inner* loss is always L2
- $\beta^{[m]}$ is found via **line search** or fixed to a **small constant value** and combined with the leaf values $c_t^{[m]}$ for tree base learners: $\tilde{c}_t^{[m]} = \beta^{[m]} \cdot c_t^{[m]}$

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

- **Feature and data subsampling** for each base learner fit
- **Parallelization** and **approximate split finding** for tree base learners
- GPU acceleration

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**

GRADIENT BOOSTING – IMPLEMENTATION

Gradient Tree Boosting

- **R:** mlr3 learners `LearnerClassifXgboost / LearnerRegrXgboost`, `LearnerClassifLightGBM / LearnerRegrLightGBM`
- **Python:** `GradientBoostingClassifier / GradientBoostingRegressor` from package `scikit-learn`, `XGBClassifier / XGBRegressor` from package `xgboost`, `lgb.train` from package `lightgbm`

⇒ LightGBM current state-of-the-art but slightly more complicated to use than xgboost

Componentwise Gradient Boosting

- **R:** `mboost` from package `mboost`, `boostLinear / boostSplines` from package `compboost`
- **Python:** /

⇒ `mboost` very flexible but slow while `compboost` is much faster with limited features

GRADIENT BOOSTING – PROS & CONS

Advantages

- + Retains 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

Disadvantages

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

LINEAR SVM – METHOD SUMMARY

CLASSIFICATION

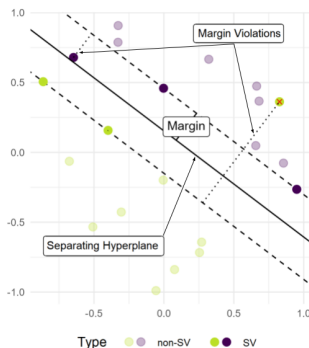
REGRESSION

PARAMETRIC

WHITE-BOX

General 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

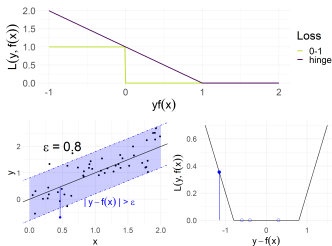
Hypothesis space (primal) $\mathcal{H} = \{f(\mathbf{x}) : f(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^\top \mathbf{x} + \theta_0)\}$

LINEAR SVM – METHOD SUMMARY

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

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

- $\|\boldsymbol{\theta}\| = 1/\gamma$ ($\hat{=}$ 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): $L(y, f) = \max(|y - f| - \epsilon, 0)$



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 $\alpha_i \geq 0$:

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle \quad \text{s.t.} \quad 0 \leq \alpha_i \leq C \quad \forall i \in \{1, \dots, n\} \quad \text{and} \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0$$

Hypothesis space (dual) Non-SVs have $\alpha_i = 0$ as they do not affect the hyperplane

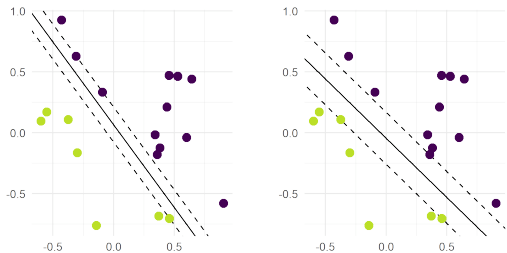
$$\mathcal{H} = \left\{ f(\mathbf{x}) : f(\mathbf{x}) = \text{sign} \left(\sum_{i=1}^n \alpha_i y^{(i)} \langle \mathbf{x}^{(i)}, \mathbf{x} \rangle + \theta_0 \right) \mid \alpha_i \geq 0, \sum_{i=1}^n \alpha_i y^{(i)} = 0 \right\}$$

LINEAR SVM – METHOD SUMMARY

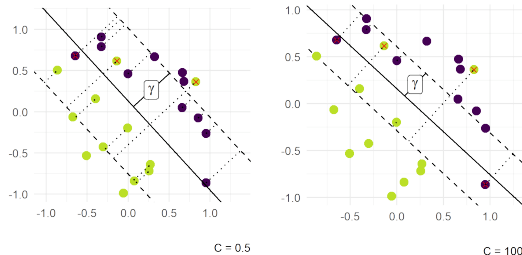
Optimization

- 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 to control maximization of the margin vs. minimizing margin violations



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



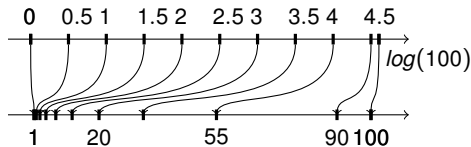
Soft-margin SVM: large margin and few margin violations on the right (best trade-off)

LINEAR SVM – IMPLEMENTATION & PRACTICAL HINTS

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



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

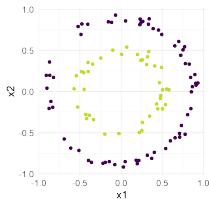
General idea

- 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**: $\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle = k(\mathbf{x}, \tilde{\mathbf{x}})$

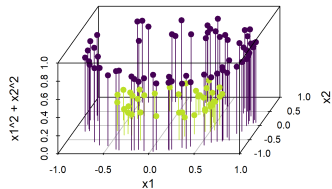
Hypothesis space

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

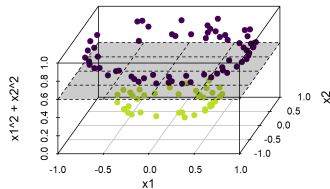
$$\mathcal{H} = \left\{f(\mathbf{x}) : f(\mathbf{x}) = \text{sign}\left(\sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0\right) \mid \alpha_i \geq 0, \sum_{i=1}^n \alpha_i y^{(i)} = 0\right\} \text{ (dual)}$$



Nonlinear problem in original space



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



NONLINEAR SVM – METHOD SUMMARY

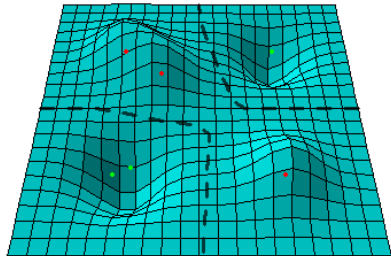
Dual problem **Kernelize** dual (soft-margin) SVM problem, replacing all inner products by kernels:

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

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

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**
→ $\beta_j = 0$ 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 $\Rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x}^\top \tilde{\mathbf{x}} \Rightarrow$ linear SVM
- **Polynomial** kernel of degree $d \in \mathbb{N}$: monomials (i.e., feature interactions) up to d -th order
 $\Rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^\top \tilde{\mathbf{x}} + b)^d, b \geq 0$
- **Radial basis function (RBF)** kernel: infinite-dimensional feature space, allowing for perfect separation of all finite datasets $\Rightarrow k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\gamma \|\mathbf{x} - \tilde{\mathbf{x}}\|_2^2)$ 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

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

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

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)

GAUSSIAN PROCESSES (GP) – METHOD SUMMARY

REGRESSION

CLASSIFICATION

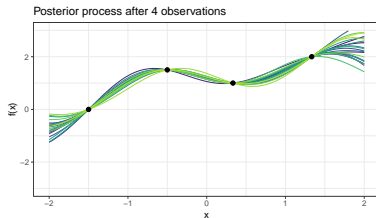
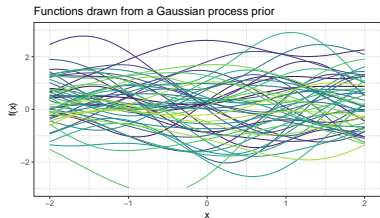
NONPARAMETRIC

PROBABILISTIC

General idea

- GPs model a distribution over potential functions f that fit the observed data
- **Assumptions:**
 - n -observations follow a n -dimensional Normal distribution
 - The closer observations are, the higher they are correlated
- A **kernel** function $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ quantifies the similarity between two observations and induced the covariance matrix of the distribution.
- **Predict** via the maximum a-posteriori (MAP) estimate.

Hypothesis space $\mathcal{H} = \left\{ f = \left[f(\mathbf{x}^{(1)}), \dots, f(\mathbf{x}^{(n)}) \right] \sim \mathcal{N}(\mathbf{m}, \mathbf{K}) \mid \mathbf{m} \in \mathbb{R}^n, \mathbf{K} \in \mathbb{R}^{n \times n} \right\}$



GAUSSIAN PROCESSES (GP) – METHOD SUMMARY

Empirical risk

- The risk is estimated by using the posterior of a conditional Normal distribution
- Most kernels have **length scale parameters** that need to be estimated

Optimization

- The kernel parameters can be learned using **maximum likelihood** estimation
- This requires inverting the $n \times n$ -covariance matrix

Hyperparameters

- The most important hyperparameter is the choice of the kernel function $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$
- Common kernel choices for "*standard*" data are:
 - Linear or polynomial
 - Squared-exponential (infinitely differentiable)
 - Matérn (further generalization of the Squared-exponential kernel)
- Special kernels for all kind of data situation exist, e.g., a Exp-Sine-Squared kernel for periodic data
- Kernels can be composed by multiplying or addition to create more expressive structures

GP – IMPLEMENTATION & PRACTICAL HINTS

Scalable GPs for larger data

- Low-rank approximations of the covariance by using only a representative subset of **inducing points**
- Using a kernel that creates a sparse covariance matrix

Noisy GPs

- Having an interpolator might not be suitable if the data is noisy
- A noisy GP adds a **nugget** effect to the kernel $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) + \sigma \delta_{ij}$, creating a Gaussian process regression model

Implementation

- **R:** `mlr3` learners `LearnerClassifGausspr / LearnerRegrGausspr`, calling `kernlab::gausspr()`
- **Python:** `GaussianProcessClassifier / GaussianProcessRegressor` from package `scikit-learn`, `gpytorch` for a modular, scalable, efficient and GPU accelerated implementation built on `torch`

GAUSSIAN PROCESSES (GP) – PROS & CONS

Advantages

- + GPs allow to **quantify prediction uncertainty** induced by both intrinsic noise in the problem and errors in the parameter estimation process
- + A GP is a function **interpolator** and will predict the exact value of a training point
- + The choice of kernel function allows considerable flexibility for problem specific characteristics
- + Automatic relevance determination (ARD) determines the importance of features

Disadvantages

- GPs are **not sparse**, i.e., they require the full training data for prediction
- GP training requires $\mathcal{O}(n^3)$, i.e., it scales cubically in the number of observations
- GPs cannot handle categorical features.
- GPs are **not particularly easy to understand** conceptually

NEURAL NETWORKS – METHOD SUMMARY

REGRESSION

CLASSIFICATION

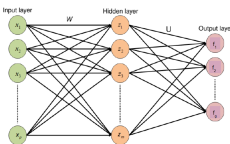
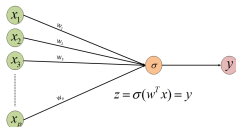
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BLACK-BOX

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



NEURAL NETWORKS – METHOD SUMMARY

Architecture

- Input layer: original features \mathbf{x}
- Hidden layers: nonlinear transformation of previous layer $\phi^{(h)} = \sigma^{(h-1)}(\phi^{(h-1)})$
- Output layer: number of output neurons and activation depends on problem $\tau(\phi)$
 - Regression: one output neuron, $\tau = \text{identity}$
 - Binary classification: one output neuron, $\tau = \frac{1}{1 + \exp(-\theta^\top \mathbf{x})}$ (logistic sigmoid)
 - Multiclass Classification: g output neurons, $\tau_j = \frac{\exp(f_j)}{\sum_{j=1}^g \exp(f_j)}$ (softmax)

Empirical risk In general, compatible with any differentiable loss

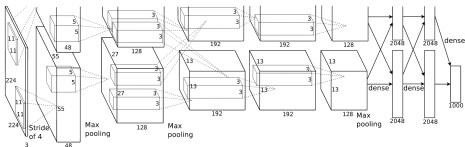
Optimization

- Variety of different optimizers, mostly based on some form of **stochastic gradient descent (SGD)**
- Improvements:
 - (1) Accumulation of previous gradients \rightarrow **Momentum**
 - (2) Weight specific scaling based on previous squared gradients \rightarrow **RMSProb**
 \Rightarrow **ADAM** combines (1) and (2)
 - (3) Learning rate schedules, e.g., decaying or cyclical learning rates
- Training progress is measured in full passes over the full training data, called **epochs**
- **Batch size** is a hyperparameter and limited by input data dimension

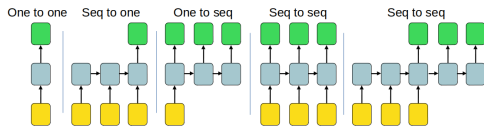
NEURAL NETWORKS – METHOD SUMMARY

Network types Large variety of architectures for different data modalities

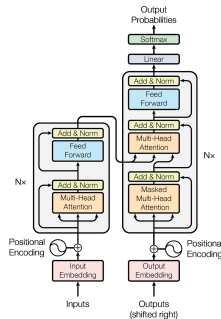
- **Feedforward NNs / multi-layer perceptrons (MLPs)**: sequence of **fully-connected** layers \Rightarrow tabular data
- **Convolutional NNs (CNNs)**: sequence of feature map extractors with spatial awareness \Rightarrow images, time series
- **Recurrent NNs (RNNs)**: handling of sequential, variable-length information \Rightarrow times series, text, audio
- **Transformers**: Learning invariances from data, handling multiple/any data modalities



Convolutional network architecture



Recurrent network architecture



Transformer network architecture

NEURAL NETWORKS – METHOD SUMMARY

Hyperparameters

- **Architecture:**

- Lots of design choices \Rightarrow tuning problem of its own.
- Typically: hierarchical optimization of components (cells) and macro structure of network
 \rightarrow **Neural Architecture Search (NAS)**
- Many predefined (well working) architectures exist for standard tasks

- **Training:**

- Initial learning rate and various regularization parameters
- Number of epochs is determined by **early-stopping**
- **Data-augmentation**, e.g., applying random rotations to input images

Foundation models

- **Enormous** models trained on vast amounts of (general) data, e.g., all of wikipedia, in **self-supervised** fashion
- Used as starting point (**pre-trained**) and fine-tuned via **transfer** or **few-shot** learning for other tasks requiring little data
- Examples: GPT-3 for language, CLIP for vision-language, ...

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
 - `PyTorch` for flexible design with a focus on research
 - `TensorFlow` for flexible design with a focus on deployment / industry
 - `huggingface` for pre-trained / foundation models

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