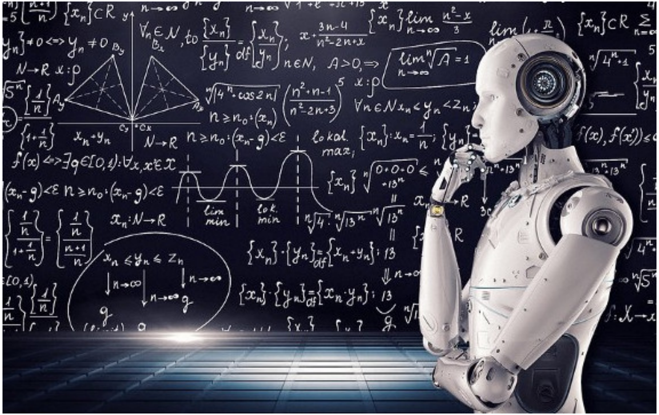
Common Machine Learning Algorithms



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CONTENTS

LINEAR MODELS

LINEAR MODELS – FUNCTIONALITY

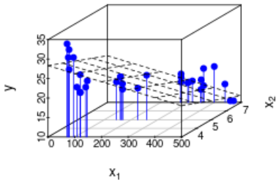
SUPERVISED | REGRESSION | CLASSIFICATION | PARAMETRIC | WHITE-BOX

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

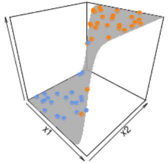
Hypothesis space

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

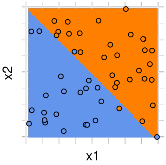
- Identity $\phi(\boldsymbol{\theta}^\top \mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x} \;\Rightarrow$ **linear regression**
- Logistic sigmoid function $\phi(\boldsymbol{\theta}^T \mathbf{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^T \mathbf{x})} =: \pi(\mathbf{x} \mid \boldsymbol{\theta}) \;\Rightarrow$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



Linear regression hyperplane



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



Corresponding separating hyperplane

LINEAR MODELS – FUNCTIONALITY

Empirical risk

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

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

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

Optimization

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

Hyperparameters None

LINEAR MODELS – PRO'S & CON'S

Advantages

+ **simple and fast** implementation
+ **analytical** solution
+ **cheap** computation
+ applicable for any **dataset size**, as long as number of observations $\gg$ number of features
+ flexibility **beyond linearity** with polynomials, trigonometric transformations etc.
+ intuitive **interpretability** via feature effects
+ statistical hypothesis **tests** for effects available

Disadvantages

— **nonlinearity** of many real-world problems
— further restrictive **assumptions**: linearly independent features, homoskedastic residuals, normality of conditional response
— **sensitivity** w.r.t. outliers and noisy data (especially with L2 loss)
— risk of **overfitting** in higher dimensions
— feature **interactions** must be handcrafted, so higher orders practically infeasible
— no handling of **missing** data

Simple method with good interpretability for linear problems, but with strong assumptions and limited complexity

LINEAR MODELS – PRACTICAL HINTS

Implementation

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

REGULARIZED LINEAR MODELS

REGULARIZED LM – FUNCTIONALITY

General idea

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

Empirical risk

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

Optimization

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

Hyperparameters Shrinkage parameter λ

REGULARIZED LM – PRACTICAL HINTS

Choice of regularization parameter

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

Ridge vs. LASSO

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

Implementation

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

LINEAR SUPPORT VECTOR MACHINES

LINEAR SVM – FUNCTIONALITY

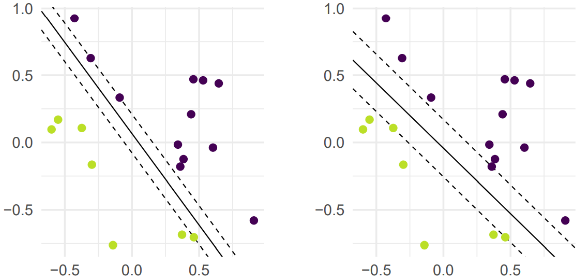
SUPERVISED CLASSIFICATION PARAMETRIC BLACK-BOX

General idea

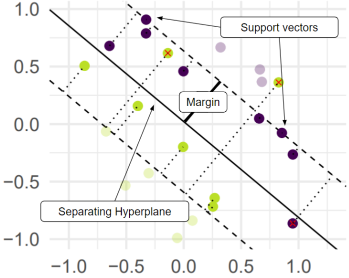
- Find linear decision boundary (**separating hyperplane**) that best separates classes
  - **Hard-margin** SVM: maximize distance (**margin** $\gamma > 0$) to closest members (**support vectors, SV**) on each side of decision boundary
  - **Soft-margin** SVM: relax separation to allowing margin violations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

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

LINEAR SVM – FUNCTIONALITY



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



Soft-margin SVM with margin violations

Dual problem

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

LINEAR SVM – FUNCTIONALITY

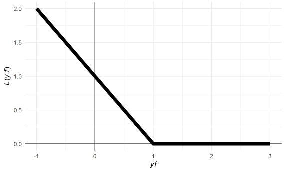
Empirical risk

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

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

with

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



Optimization Non-differentiable problem $\rightarrow$ mostly **sub-gradient** methods

Hyperparameters Cost parameter C

LINEAR SVM – PRO'S & CON'S

Advantages

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

Disadvantages

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

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

LINEAR SVM – PRACTICAL HINTS

Preprocessing

Features must be rescaled before applying SVMs.

Tuning

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

Implementation

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