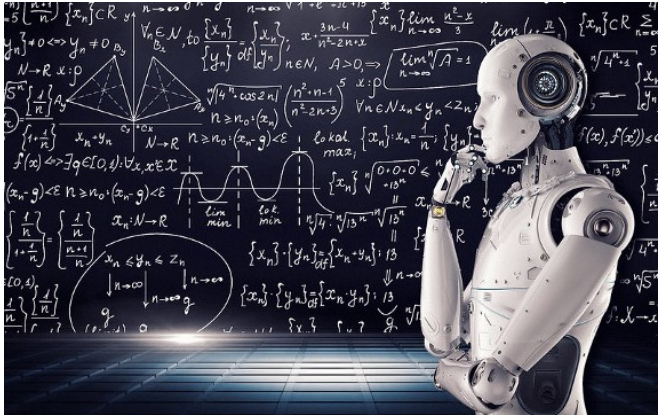
Common Machine Learning Algorithms



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LINEAR MODELS

LINEAR MODELS – FUNCTIONALITY

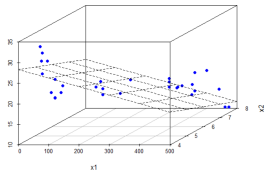
SUPERVISED | PARAMETRIC | WHITE-BOX

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

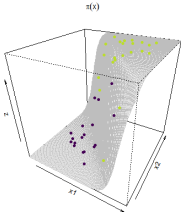
Hypothesis space

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

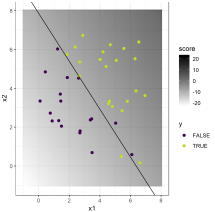
- Identity $\phi(\boldsymbol{\theta}^\top \mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x}$ $\Rightarrow$ **linear regression**
- Logistic sigmoid function $\phi(\boldsymbol{\theta}^T \mathbf{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^T \mathbf{x})} =: \pi(\mathbf{x} \mid \boldsymbol{\theta})$ $\Rightarrow$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



Separating hyperplane for bivariate logistic regression

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** with more flexible feature transformations (e.g., high-degree polynomials)
- — 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`

Regularization

- Quadratic penalty on model coefficients (a.k.a. **Ridge** regression)
  - Overall smaller, but still dense θ
  - Suitable with many influential features present, handling correlated features by shrinking their coefficients equally
- Absolute penalty on model coefficients (a.k.a. **Lasso** regression)
  - Actual variable selection
  - Suitable for sparse problems, ineffective with correlated features (randomly selecting one)
- Weighted combination of Ridge and Lasso: **elastic net**