BABD

INTERNATIONAL MASTER IN BUSINESS ANALYTICS AND BIG DATA

Supervised Learning - Regression

MIP POLITECNICO DI MILANO GRADUATE SCHOOL OF BUSINESS

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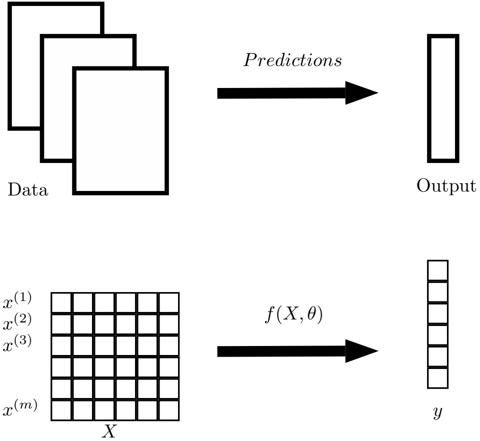
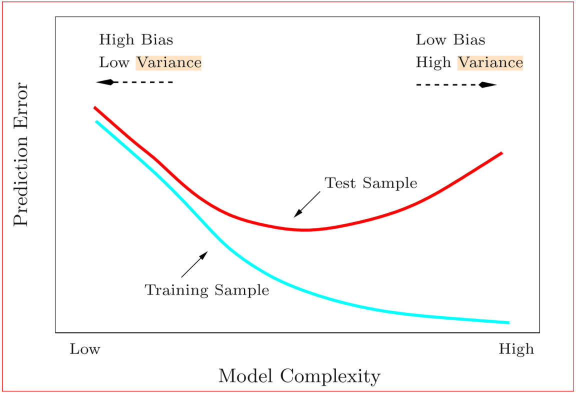
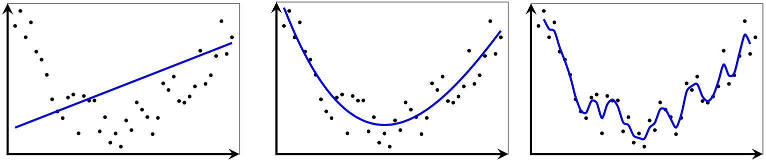
Supervised Learning



Under/Over-fitting





Underfitting   Balance   Overfitting

Quality measures - Regression

- Coefficient of determination

$$R^2 = 1 - \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / \sum_i (y_i - \bar{y})^2$$

- Mean Absolute Error :

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|$$

- Mean Squared Error :

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- Root Mean Squared Error : $RMSE = \sqrt{MSE}$

Regression model

- Dataset $\mathcal{D}$ contain m observation/records and $n+1$ attributes.
- n independent features and a single continuous dependent attribute: target
- We can represent our dataset as a numeric matrix X of dimension $m \times n$
- Our aim is to find a function $f : \mathbb{R}^n \to \mathbb{R}$ such that the *associated error* to our prediction

$$\hat{y} = f(x_1, x_2, \ldots, x_n)$$

is small

Regression models

- **linear**

$$Y = w_1 X_1 + w_2 X_2 + \cdots + w_n X_n + b = \sum_{j=1}^{n} w_j X_j + b.$$

- **quadratic**

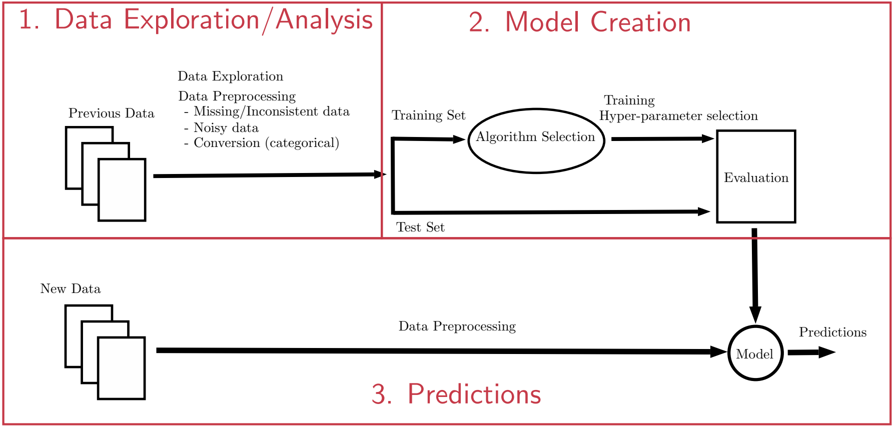
$$Y = b + wX + dX^2 \qquad Z = X^2$$

$$Y = b + wX + dZ.$$

- **exponential**

$$Y = e^{b+wX} \qquad Z = \log Y \qquad Z = b + wX.$$

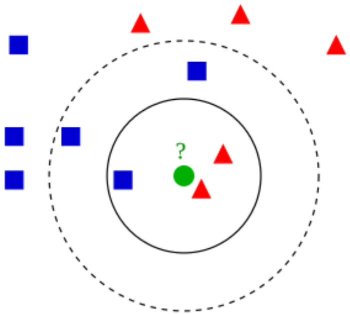
Supervised Learning Workflow



Regression Models

- Heuristics Methods
  - Nearest Neighbours
  - Regression Trees
- Optimization based Methods
  - Support vector machine
  - Neural Networks
  - Linear models

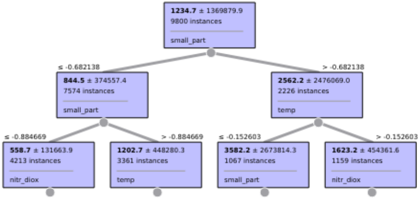
KNN K-nearest Neighbours



Main Parameters

- k : number of neighbours
- neighbour weights
- distances

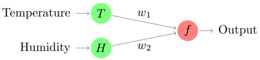
Regression tree

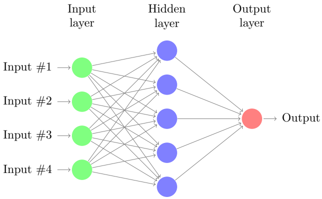


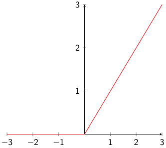
Main Parameters

- variability measure: mse (variance from mean), mae (error from median)
- max_depth
- min_samples_split: minimum number of samples to split an internal node
- min_sample_leaf: minimum number of samples required to be at a leaf node

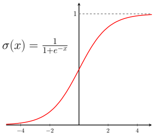
Multi-Layer Perceptron







ReLU

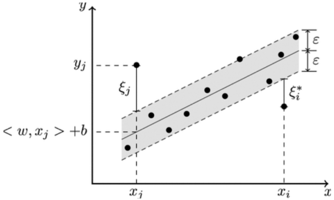


Sigmoid

Main Parameters

- hidden_layer_sizes: $(n_1, n_2, \ldots, n_L)$
- activation: identity, logistic, tanh, relu
- alpha regularization term parameter
- Resolution algorithm parameters: solver, tol, batch_size, learning_rate, max_iter.

SVR



$$\min_{w,b,\zeta,\zeta^*} \frac{1}{2}\|w\| + C\sum_{i=1}^{n}(\zeta_i + \zeta_i^*)$$

$$\begin{aligned} \text{subject to } & y_i - w^T\phi(x_i) - b \leq \varepsilon + \zeta_i, \\ & w^T\phi(x_i) + b - y_i \leq \varepsilon + \zeta_i^*, \\ & \zeta_i, \zeta_i^* \geq 0, i = 1, ..., n \end{aligned}$$

Main Parameters

- C: inverse of regularization strength
- ε: tolerance
- kernel
- Resolution algorithm parameters

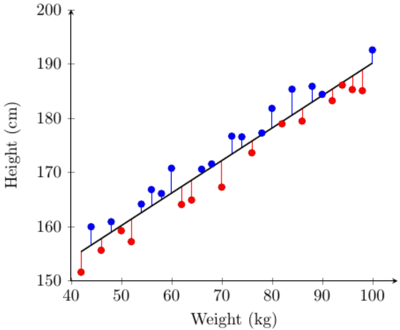
Simple linear regression

- Deterministic model

$$Y = w\,X + b$$

- Probabilistic model

$$Y = w\,X + b + \varepsilon$$



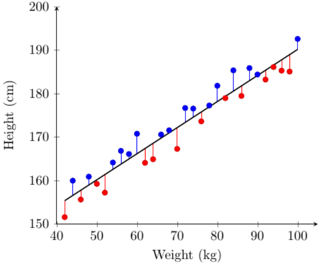
Simple linear regression

- Residuals

$$e_i = y_i - f(x_i) = y_i - wx_i - b \qquad i \in \mathcal{M}$$

- Least square regression

$$SSE = \sum_{i=1}^{m} e_i^2 = \sum_{i=1}^{m} [y_i - wx_i - b]^2$$



Least square regression

- **find the minimum**

$$\frac{\partial\,\mathrm{SSE}}{\partial b} = -2\sum_{i=1}^{m}[y_i - wx_i - b] = 0,$$

$$\frac{\partial\,\mathrm{SSE}}{\partial w} = -2\sum_{i=1}^{m} x_i[y_i - wx_i - b] = 0.$$

- **normal equation (linear system depending from the coefficients)**

$$\begin{pmatrix} m & \sum_{i=1}^{m} x_i \\ \sum_{i=1}^{m} x_i & \sum_{i=1}^{m} x_i^2 \end{pmatrix} \begin{pmatrix} b \\ w \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{m} y_i \\ \sum_{i=1}^{m} x_i y_i \end{pmatrix}$$

Least square linear regression

- $$\hat{w} = \frac{\sigma_{xy}}{\sigma_{xx}},$$
  $$\hat{b} = \bar{\mu}_y - \hat{w}\bar{\mu}_x,$$

- $$\bar{\mu}_x = \frac{\sum_{i=1}^{m} x_i}{m}, \qquad \bar{\mu}_y = \frac{\sum_{i=1}^{m} y_i}{m},$$

  $$\sigma_{xy} = \sum_{i=1}^{m} (x_i - \bar{\mu}_x)(y_i - \bar{\mu}_y),$$
  $$\sigma_{xx} = \sum_{i=1}^{m} (x_i - \bar{\mu}_x)^2,$$
  $$\sigma_{yy} = \sum_{i=1}^{m} (y_i - \bar{\mu}_y)^2,$$

Least square multiple linear regression

- **probabilistic model**

$$Y = w_1 X_1 + w_2 X_2 + \cdots + w_n X_n + b + \varepsilon.$$

$$\mathbf{e} = (e_1, e_2, \ldots, e_m)$$

$$\mathbf{w} = (b, \mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_n)$$

- **extend matrix X by a vector with all components = 1**

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}.$$

Least square multiple linear regression

- **sum of squared residuals**

$$\mathrm{SSE} = \sum_{i=1}^{m} e_i^2 = \|\mathbf{e}\|^2 = \sum_{i=1}^{m} (y_i - \mathbf{w}'\mathbf{x}_i)^2$$
$$= (\mathbf{y} - \mathbf{X}\mathbf{w})'(\mathbf{y} - \mathbf{X}\mathbf{w}).$$

- **null partial derivatives**

$$\frac{\partial\, \mathrm{SSE}}{\partial \mathbf{w}} = -2\mathbf{X}'\mathbf{y} + 2\mathbf{X}'\mathbf{X}\mathbf{w} = \mathbf{0}.$$

- **normal equation**

$$\mathbf{X}'\mathbf{X}\mathbf{w} = \mathbf{X}'\mathbf{y}.$$

- **minimum point**

$$\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}.$$

Linear Models generalizations

- Regularization

$$\min_{\mathbf{w}} RR(\mathbf{w}, \mathcal{D}) = \min_{\mathbf{w}} \lambda \|\mathbf{w}\|^2 + \sum_{i=1}^{m} (y_i - \mathbf{w}'\mathbf{x}_i)^2$$
$$= \min_{\mathbf{w}} \lambda \|\mathbf{w}\|^2 + (\mathbf{y} - \mathbf{X}\mathbf{w})'(\mathbf{y} - \mathbf{X}\mathbf{w}).$$

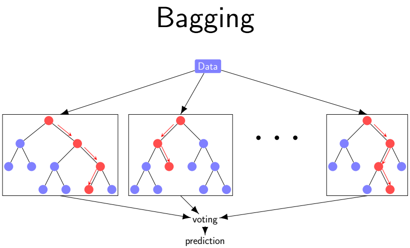
$$\min_{\mathbf{w}} LR(\mathbf{w}, \mathcal{D}) = \min_{\mathbf{w}} \lambda \,|\mathbf{w}| + \sum_{i=1}^{m} (y_i - \mathbf{w}'\mathbf{x}_i)^2$$
$$= \min_{\mathbf{w}} \lambda \,|\mathbf{w}| + (\mathbf{y} - \mathbf{X}\mathbf{w})'(\mathbf{y} - \mathbf{X}\mathbf{w}).$$

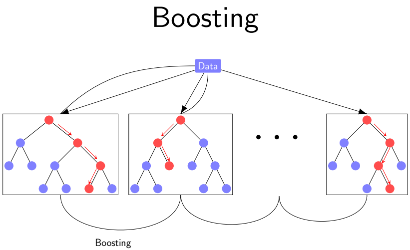
- General Linear Models
  - **Functions g_h represent any set of bases, such as polynomials, kernels and other groups of nonlinear functions**

$$Y = \sum_{h} w_h g_h(X_1, X_2, \ldots, X_n) + b + \varepsilon$$

  - **Coefficients w_h and b can be determined through the minimization of the sum of squared errors. Function SSE in this formulation is more complex than for linear regression, solution of the minimization problem more difficult**

Ensemble Methods





Residual assumptions

- values predicted by model

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = (\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}')\mathbf{y} = \mathbf{H}\mathbf{y}$$

- hat matrix

$$\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$$

- residuals

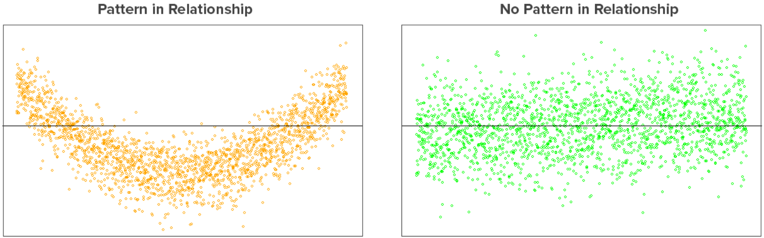
$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = (\mathbf{I} - \mathbf{H})\mathbf{y}.$$

Residual assumptions

$$\mathrm{E}(\varepsilon_i|\mathbf{x}_i) = 0,$$
$$\mathrm{Var}(\varepsilon_i|\mathbf{x}_i) = \sigma^2$$

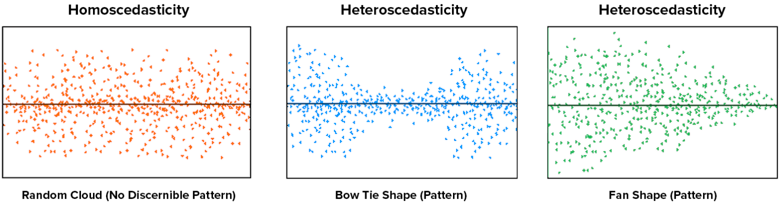
- residuals ε_j e ε_k should be independent
- estimate of σ $$\bar{\sigma}^2 = \frac{\mathrm{SSE}}{m-n-1} = \frac{\sum_{i=1}^{m}(y_i - \mathbf{w}'\mathbf{x}_i)^2}{m-n-1} = \frac{\mathbf{y}'(\mathbf{I}-\mathbf{H})\mathbf{y}}{m-n-1},$$
- if standard deviation σ is constant we have homoscedasticity, otherwise heteroscedasticity

Residual assumptions



Residual assumptions

- Graphical distribution



- Graphically compare error distribution against a normal distribution with QQ-plots
- Apply an hypothesis test to check the normality of the errors (Kolmogorov–Smirnov, D'Agostino, etc.)