Machine Learning

Supervised learning 2

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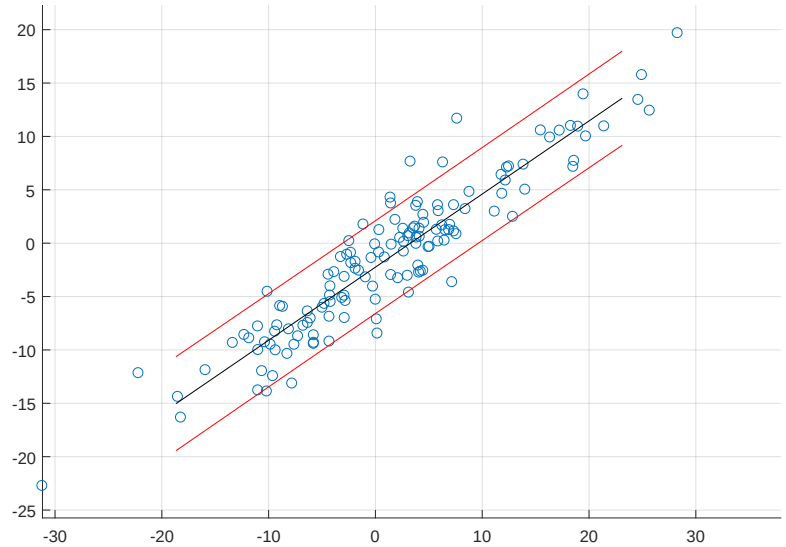
Linear regression: probably the oldest machine learning technique



- Find linear correlation coefficient.
- Compute coefficients of the linear equation

$$\hat{y} = ax + b$$

- Evaluate the model

- In multivariate case it is required to identify coefficients of the model

$$\hat{y} = a_1 x_1 + a_2 x_2 + \ldots + a_n x_n + b.$$

This leads the necessity to choose variables (perform model building).

Linear regression

- Correlation coefficient.

$$\rho = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

  where, n - is the sample size, x and y are the variable of interest.

- $-1 \leq \rho \leq 1$
- Assumption there are exist α and β such that for any $i = 1, \ldots, n$ $y_i = \alpha x_i + \beta + \varepsilon_i$ holds. Assumption: ε is sufficiently small normally distributed.
- The goal of regression is to find estimates of the coefficients α and β, such that for a and b

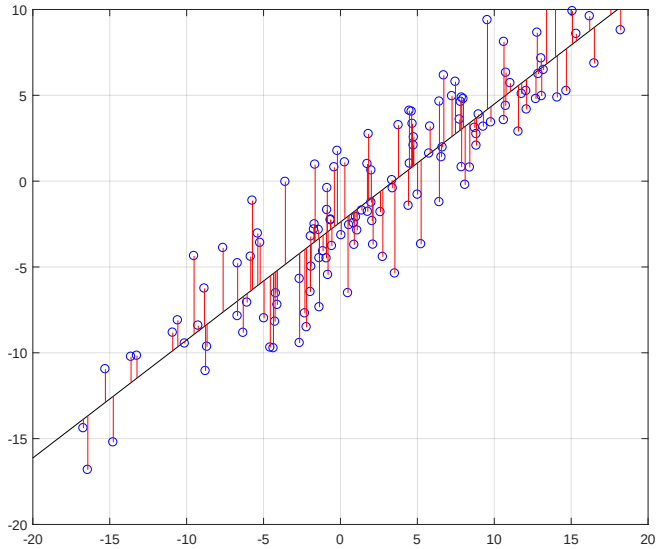
$$y_i = ax_i + b + \hat{\varepsilon}_i$$

  sum of squares of $\hat{\varepsilon}_i$ would be minimal. NB! notation $\hat{\alpha}$ and $\hat{\beta}$ is also widely use.

Least squares method

Least squares method:

$$a = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}; \quad b = \bar{y} - a\bar{x}$$



For an arbitrary number of variables:

$$y = b_1 x_1 + \ldots + b_n x_n + b_0$$

then

$$\hat{b} = (X^T X)^{-1} X^T y.$$

where each row of matrix X is input vector with 1 in the first position.

Model validation

- Coefficient of determination R^2 and adjusted R^2.
- Significance of the model and model coefficients.
- Verify assumption that residuals are normally distributed.
- Residual sum squares. $\mathrm{RSS} = \sum_{i=1}^{N}(y_i - x_i^T\beta)^2$.
- Sum squares of the regression $\mathrm{SSR} = \sum_{i=1}^{N}(\hat{y}_i - \bar{y})^2$.
- Total sum squares or sum of squares about the mean $\mathrm{SST} = \sum_{i=1}^{N}(y_i - \bar{y})^2$.
- R^2 computed as the ratio of Sum squares of the regression to total sum squares or one minus ratio of Residual sum squares to total sum squares whereas adjusted R^2 is one minus ratio of residual sum squares computed for $n-1$ to Total sum squares for $n-p$ observation points.

MLE for regression least squares I

- Linear regression is the model of the form

$$p(y|x,\theta) = \mathcal{N}(y|\beta^T x, \sigma^2)$$

  where β are the coefficients of the linear model, σ is the standard deviation of x and $\theta = (\beta, \sigma^2)$
- Parameter estimation of a statistical model is usually performed by computing MLE $\hat{\theta} = \arg\max_\theta \log p(\mathcal{D}|\theta)$. remind that $\mathcal{D}$ denotes the data set

MLE for regression least squares II

- Assumption: elements of the training set are independent and identically distributed.
- Then log likelihood is given by $\ell(\theta) = \log p(\mathcal{D}|\theta) = \sum_{i=1}^{N} \log p(y_i|x_i, \theta)$.
- As usually instead of maximizing the log- likelihood one may minimize negative log likelihood.
-

$$\ell(\theta) = \sum_{i=1}^{N} \log \left[\left(\frac{1}{2\pi\sigma^2} \right) \exp\left(-\frac{1}{2\sigma^2} (y_i - \beta^T x_i)^2 \right) \right]$$

$$= \frac{-1}{2\sigma^2} \mathrm{RSS}(\beta) - \frac{N}{2} \log(2\pi\sigma^2).$$

MLE for regression least squares II

- In order to minimize RSS differentiate its equation which lead

$$\nabla\theta = X^T X\beta - X^T y.$$

- Equate it to zero and solve for β

$$\beta = (X^T X)^{-1} X^T Y$$

last equation is referred as normal equation.

Regularization

- Overfitting may be caused by the fact that chosen model structure and data are not conform on another.
- Regularization is the technique used to overcome overfitting.
- Regularization imposes cost or penalty on the cost function and prevent larger values of the coefficients.
- Loosely speaking, regularization shrinks the coefficients towards zero and towards one another.

Ridge regression

- Ridge regression shrinks the coefficients by penalizing their size.

$$\hat{\beta}^{\text{ridge}} = \text{argmin}_{\beta}\left\{\sum_{i=1}^{N}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2\right\}$$

  λ is the nonnegative shrinkage parameter, its large values correspond to the greater amount of shrinkage applied.

- Alternatively the following notation is widely used:

$$\begin{aligned}\hat{\beta}^{\text{ridge}} &= \text{argmin}_{\beta}\sum_{i=1}^{N}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 \\ &\text{subject to} \quad \sum_{j=1}^{N}\beta_j^2 \leq t\end{aligned}$$

The Lasso

- Ridge regression shrinks the coefficients by penalizing their size.

$$\hat{\beta}^{\text{lasso}} = \text{argmin}_{\beta} \frac{1}{2} \Big\{ \sum_{i=1}^{N} \big(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \big)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \Big\}$$

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- Computing the lasso solution is a quadratic programming problem.

Statistical hypothesis testing (brief reminder I)

- Assumption about a parameter of population is a statistical hypothesis.
- Usually a pair of hypothesis is stated (H_0, H_1), notation (H_0, H_a).
  - H_0 the null hypothesis usually states that there is no statistically significant relationship between two phenomena.
  - H_1 the alternative hypothesis usually states the opposite to the H_0.
- Choose and compute test statistic and rejection rule.
- Interpret the results.
- What can possibly go wrong?

Statistical hypothesis testing (brief reminder II)

	Accept H_0	Reject H_0
H_0 is true	Correct	Type 1 Error
H_0 is false	Type II Error	Correct

Model building (feature selection)

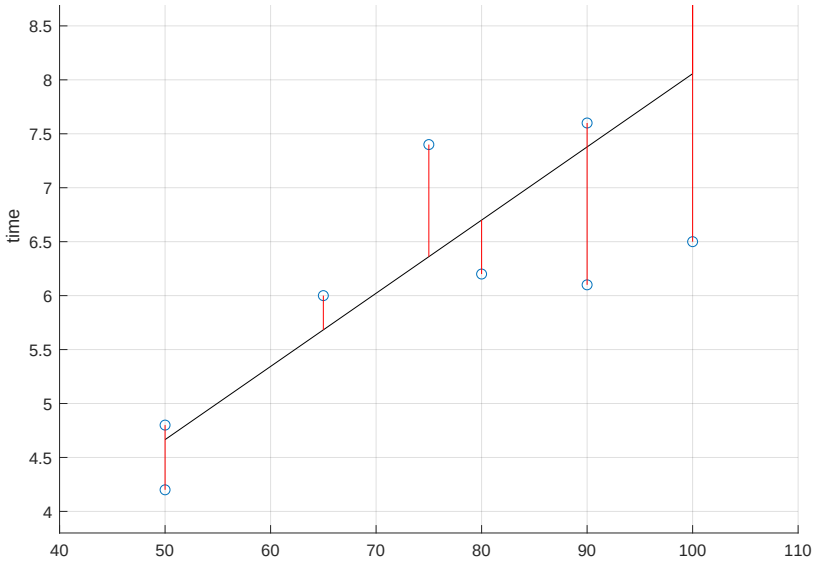
Let us suppose that observed process has p independent variables $x_1, \ldots, x_p$ and one dependent variable y. Should one build the regression equation using all p variables or not?

- Are all the variables $x_1, \ldots, x_p$ uncorrelated?
- Which subset of variables result in a "better" model?
- How to prove that as a result of adding or deleting a variable model quality has improved?

"Butler tracking company" example

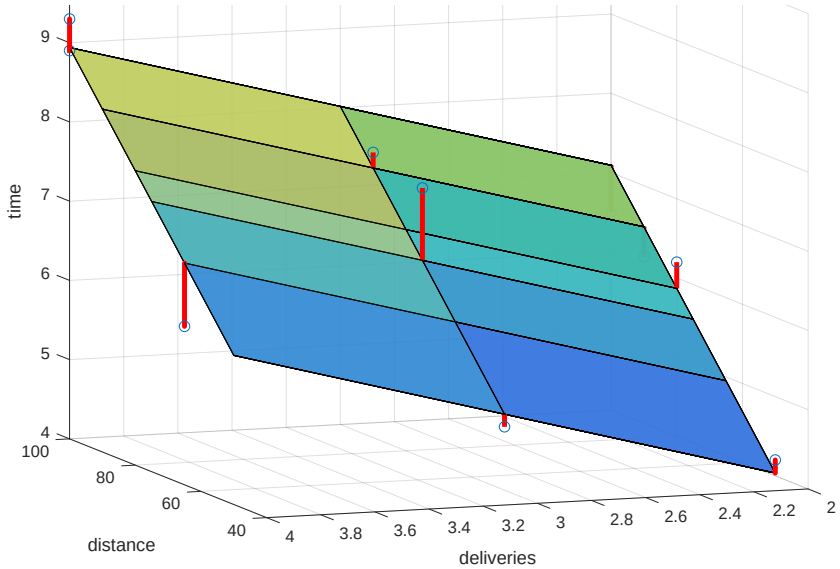
- Independent variables: Distance to drive and number of parcels to deliver. Dependent variable: time.
- Distances to drive for each assignment: 100, 50, 100, 100, 50, 80, 75, 65, 90, 90.
- Number of parcels to deliver: 4, 3, 4, 2, 2, 2, 3, 4, 3, 2
- Time in hours: $9.3, 4.8, 8.9, 6.5, 4.2, 6.2, 7.4, 6, 7.6, 6.1$.
- Pearson correlation coefficient between distance and time is 0.81.

"Butler tracking company" example continued



Model 1

Is significant $p = 0.004$, $F = 15.1846$ whereas $R^2 = 0.6641$.



Model 2

Is significant $p = 0.000276$, $F = 32.9$ whereas adjusted $R^2 = 0.87$.

Is it enough to say that model 2 is more precise?

Quality comparison

- To compare different models residual sum of squares (RSS) is used.
- Hypothesis statements: $H_0 : \mathrm{RSS}_s \leq \mathrm{RSS}_c$ $H_1 : \mathrm{RSS}_s > \mathrm{RSS}_c$.
- Test statistic (empirical parameter) for ANOVA:

$$F_{stat} = \left(\frac{\mathrm{RSS}_s - \mathrm{RSS}_c}{m} \right) \left(\frac{\mathrm{RSS}_c}{n - p - 1} \right)^{-1}$$

  where RSS_c is the residuals sum squares of model with more variables, RSS_s - is the residuals sum squares of model with less variables, m number of variables added or removed, n is the number of observation points, p - is the number of variables in more complicated model.
- Rejection rule for α (significance level), degrees of freedom: first is the number of variables added or removed, second is $n - p - 1$.
- Decision:
  - (if adding variables) rejected null hypothesis proves that adding variables caused model quality to increase significantly.
  - (if deleting variables) rejected alternative hypothesis proves that deleting variables did not cause model quality to significant decrease.

"Butler tracking company" example continued

- $\mathrm{RSS}_1 = 15.8713$, $\mathrm{RSS}_2 = 2.2994$ NB! Observe that corresponding MATLAB notation is SSE!!!
- choose $\alpha = 0.05$ degrees of freedom: first will be 1 (one variable (number of parcels)) were added, second 7 ($n = 10, p = 2$).
- Rejection rule: reject H_0 if $F_{stat} > 5.5914$
- Compute $F_{stat} = 17.4411$. (use table, or MATLAB or EXCEL)
- Reject H_0. Adding the variable has increased the model quality.

Linear model building 1

- Choose or determine all the hyperparameters. Possible order limitations, backward elimination / forward selection/ batch processing, set the level of significance and threshold for correlation. These parameters also define stopping criteria.
- Stop when: model is significant, and goodness parameters as expected OR no more variables to add or delete OR maximal or minimal order is reached etc.
- Investigate if available explanatory variables (predictors) are linearly independent. Strong dependencies between variables chosen as "independent" lead problems with inverting matrix X. Compute multicollinearity matrix where element in ith row and jth column is Pearson correlation coefficients computed for variables i and j. Based on this table determine subset(s) of variables which are linearly independent.

Linear model building 2

- Repeat
- Apply mean squares (or other technique) to build the model from selected variables.
- Evaluate significance- and quality- of the model. For quality observe determination coefficient and error. For significance use F - test and t-test variable wise.
- If model fail goodness or significance check then return to the previous model and choose another set of variables to add/delete.
- Starting from second iteration prove, using F - test, that as a result of adding/deliting variables model quality has improved/did not decreased significantly.
- If adding/deliting variables was not successful return to the previous model and if possible chose another variable(s) to add /delete or report the model from previous step.
- If goodness criteria (quality and significance) is met stop and return the model.
- If goodness criteria was not met but adding deleting variables proved to be successful chose the set of variables to be added or deleted (t-test) on the next step.
- Until stopping criteria is reached.
- Report the results.

Linear model building 3

Reminder p - is the number of variables n is the sample size.

- F -test of overall significance in regression analysis.
- Test for model significance. $H_0 : b_1 = \ldots = b_p = 0$, $H_1 : \exists i : 1 \leq i \leq p \& b_i \neq 0$.
- Test statistic:

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

- Rejection rule: Determine using F-table or corresponding software function with chosen significance level, n degrees of freedom in denominator and p degrees of freedom in nominator.

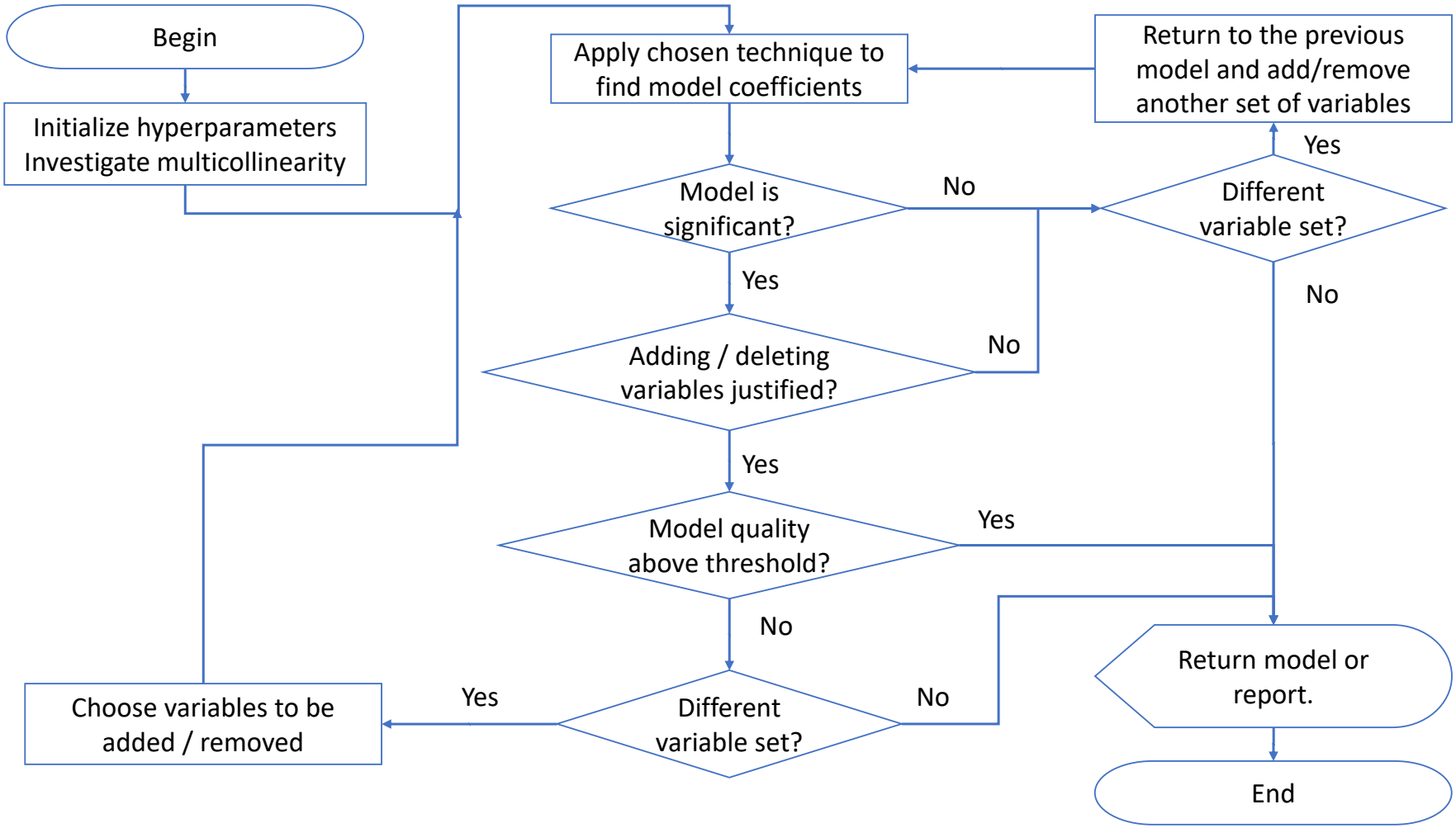
Linear model building 4

- F -test to determine significance of change in model quality caused by adding variables
  - $H_0 : RSS_S \leq RSS_C$, $H_1 : RSS_S > RSS_C$.
  - Test statistic:

$$F = \frac{\frac{RSS_S - RSS_C}{m}}{\frac{RSS_C}{n-p-1}}$$

  - Rejection rule: Determine using F-table or corresponding software function with chosen significance level, $n - p - 1$ degrees of freedom in denominator and m degrees of freedom in nominator.
- t - test on individual regression coefficients
  - $H_0 : b_i = 0$, $H_1 : b_i \neq 0$.
  - Test statistic: $t = \hat{b_i}/se(\hat{b_i})$
  - Use t - table or corresponding function to find rejection rule for chosen significance and $n - 2$ degrees of freedom.

Linear model building 5



Nonlinear regression

- By replacing independent variables X with a nonlinear mapping $\phi(X)$.
- This will lead
$$f_\theta(X) = \theta^T \phi(X)$$
- This process is referred as basis function expansion.
- Example: Polynomial regression has basis function $\phi(X) = [1, x, x^2, \ldots, x^d]$. The model remains linear in the parameters.

Polynomial regression 1

- Higher degree polynomial models tend to over fit. The coefficients become relatively large, which causes the regression curve to "wiggle".
- In order to achieve "encourage" smaller weight values introduce zero-mean Gaussian prior:

$$p(\theta) = \prod_j \mathcal{N}(\theta_j | 0, \tau^2)$$

  where $1/\tau^2$ controls the strength of prior.
- This lead following log-likelihood estimate

$$\ell = \sum_{i=1}^{N} \log \mathcal{N}(y_i | \theta^T x_i, \sigma^2) + \sum_{j=1}^{p} \log \mathcal{N}(\theta_j | 0, \tau^2)$$

- The solution is given by:

$$\hat{\theta}_r = (\lambda I + X^T X)^{-1} X^T y$$

Logistic regression

- Remind that linear regression may be written in the following form:

$$p(y|x,\theta) = \mathcal{N}(y|\mu(x),\sigma^2(x))$$

- This may be generalized to the binary setting as follows:

$$p(y|x,\theta) = \mathrm{Ber}(y|\mathrm{sigm}(\theta^T x))$$

where $\mathrm{sigm}(\eta) = (1+e^{-\eta})^{-1}$. Will be referred as logistic regression.

- Fitting is usually done by maximum likelihood

$$\ell(\theta) = \sum_{i=1}^{N} \log p_(g_i)(x_i|\theta) = \sum_{i=1}^{N} \left\{ y_i \beta^T x_i - \log(1+e^{\beta^T x_i}) \right\}$$

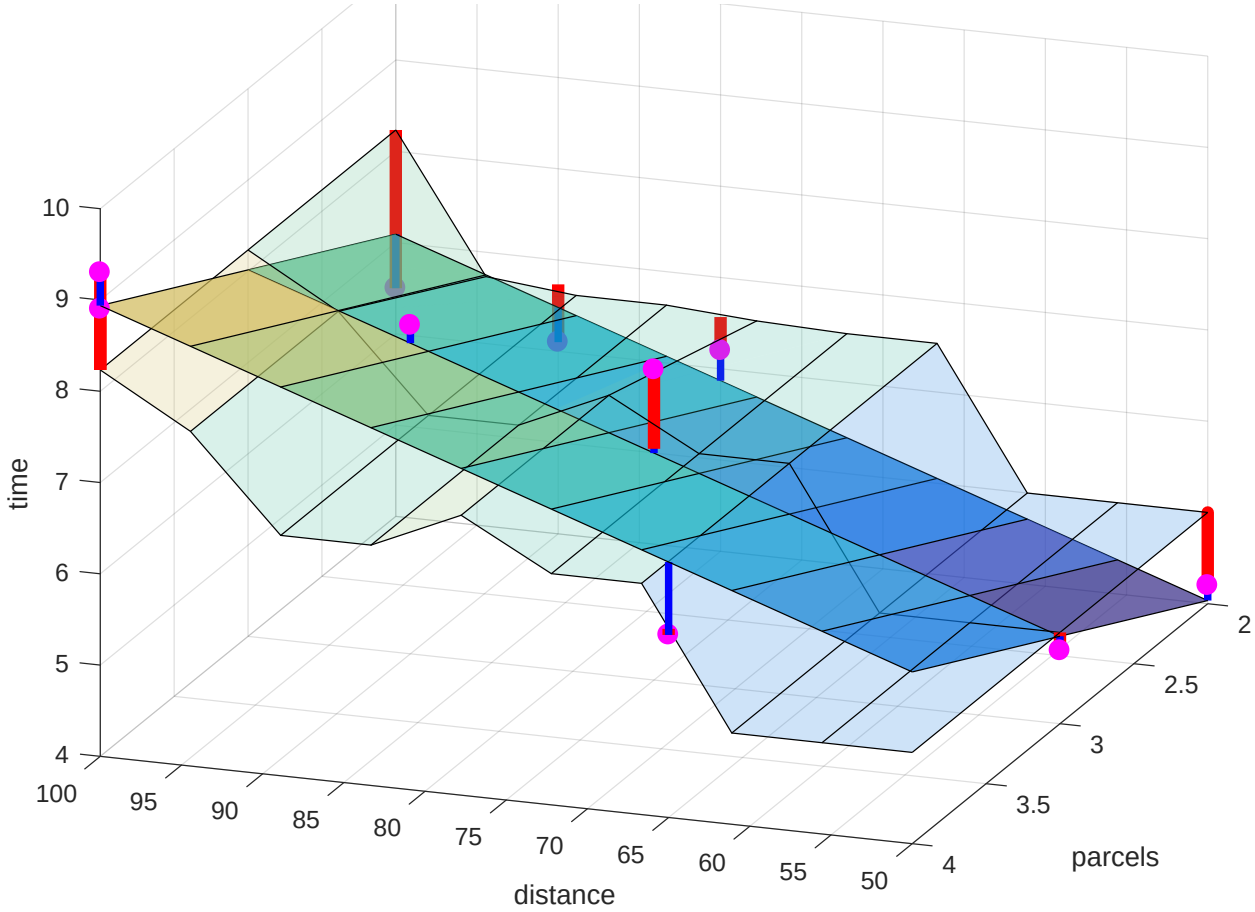
- Solving the last one is done by means of iterative algorithm.

$$\begin{aligned} b^{\text{new}} &= \arg\min_b (z - Xb)^T W (z - Xb) \\ z &= Xb + W^{-1}(y - p) \end{aligned}$$

where W is a $N \times N$ diagonal matrix with ith element $p(x_i, |b)(1 - p(x_i|b))$

k-nn regression

The value of the response (dependent variable) defined as the average of its k nearest neighbours from the training set.



Regression trees

- Partition the feature space into the set of rectangles.
- Fit a simple model (for example constant) in each rectangle.
- Fitting the model is similar to the case of classification trees.