Statistical Natural Language Processing ML intro & regression

Çağrı Çöltekin

University of Tübingen Seminar für Sprachwissenschaft

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Why machine learning?

- Majority of the modern computational linguistic tasks and applications are based on machine learning
 - Tokenization
 - Part of speech tagging
 - Parsing
 - …
 - Speech recognition
 - Named Entity recognition
 - Document classification
 - Question answering
 - Machine translation
 - ..

Machine learning is ...

The field of machine learning is concerned with the question of how to construct computer programs that automatically improve with experience.

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Statistical learning refers to a vast set of tools for understanding data.

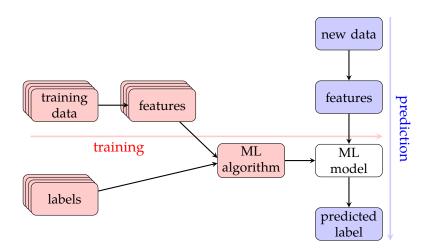
—James et al. (2013)

Supervised or unsupervised

- Machine learning methods are often divided into two broad categories: *supervised* and *unsupervised*
- Supervised methods rely on labeled (or annotated) data
- Unsupervised methods try to find regularities in the data without any (direct) supervision
- Some methods do not fit any (or fit both):
 - Semi-supervised methods use a mixture of both
 - Reinforcement learning refers to the methods where supervision is indirect and/or delayed

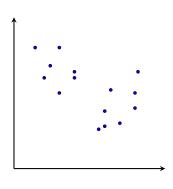
In this course, we will mostly discuss/use supervised methods.

Supervised learning



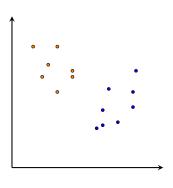
Unsupervised learning

- In unsupervised learning we do not have any labels
- The aim is discovering some 'latent' structure in the data
- Common examples include
 - Clustering
 - Density estimation
 - Dimensionality reduction
- In NLP, methods that do not require (manual) annotation are sometimes called unsupervised



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Supervised learning

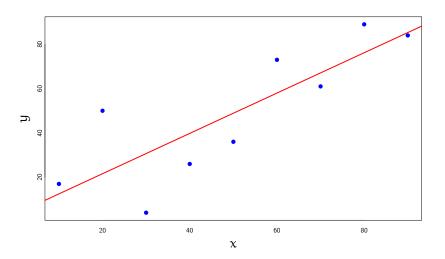
two common settings

An ML algorithm is called

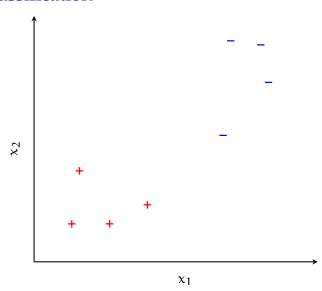
regression if the outcome to be predicted is a numeric (continuous) variable

classification if the outcome to be predicted is a categorical variable

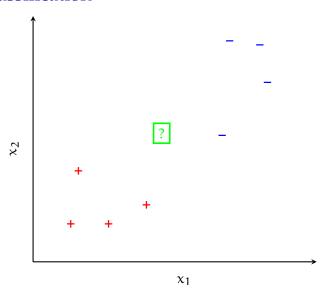
Regression



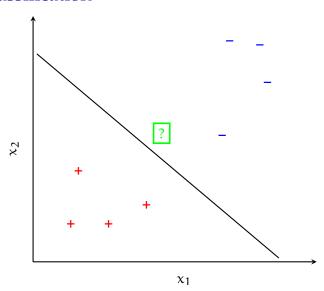
Classification



Classification



Classification



ML topics we will cover in this course

- (Linear) Regression (today)
- Classification (perceptron, logistic regression)
- Evaluation ML methods / algorithms
- Unsupervised learning
- Sequence learning
- Neural networks / deep learning

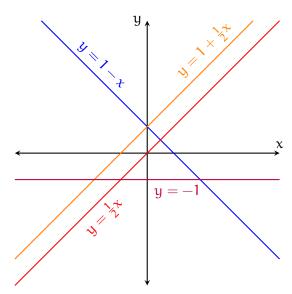
Regression

- Regression is a (supervised) method for predicting the value of a continuous response variable based on a number of predictors
- We estimate the conditional expectation of the outcome variable given the predictor(s)
- It is the foundation of many models in statistics and machine learning
- If the outcome is a label, the problem is called classification

The linear equation: a reminder

$$y = a + bx$$

- a (intercept) is where the line crosses the y axis.
- b (slope) is the change in y as x is increased one unit.



The simple linear model

$$y_i = a + bx_i + \epsilon_i$$

- y is the *outcome* (or response, or dependent) variable. The index i represents each unit observation/measurement (sometimes called a 'case')
- x is the *predictor* (or explanatory, or independent) variable
- a is the *intercept* (called *bias* in the NN literature)
- b is the *slope* of the regression line.
- a and b are called coefficients or parameters
 - a + bx is the *deterministic* part of the model. It is the model's prediction of y (\hat{y}), given x
 - ε is the residual, error, or the variation that is not accounted for by the model. Assumed to be normally distributed with 0 mean

$$y_i = a + bx_i + \epsilon_i$$

$$y_i = \alpha + \beta x_i + \epsilon_i$$

• Sometimes, Greek letters α and β are used for intercept and the slope, respectively

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

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- Another common notation to use only b, β , θ or w, but use subscripts, 0 indicating the intercept and 1 indicating the slope

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$$y_i = \hat{w}_0 + \hat{w}_1 x_i + \epsilon_i$$

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$$y_i = wx_i + \epsilon_i$$

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- Sometimes coefficients wear hats, to emphasize that they are estimates
- Often, we use the vector notation for both input(s) and coefficients: $\mathbf{w} = (w_0, w_1)$ and $\mathbf{x_i} = (1, \mathbf{x_i})$

Estimating model parameters: reminder

In least-squares regression, we find

$$\hat{\boldsymbol{w}} = \operatorname*{arg\,min}_{\boldsymbol{w}} \sum_{i} (y_i - \hat{y}_i)^2$$

In general, we define an objective (or loss) function J(w) (e.g., negative log likelihood), and minimize it with respect to the parameters

$$\hat{\boldsymbol{w}} = \operatorname*{arg\,min}_{\boldsymbol{w}} J(\boldsymbol{w})$$

Then,

- take the derivative of J(w)
- set it to 0
- solve the resulting equation(s)

Least-squares regression

$$y_i = \underbrace{w_0 + w_1 x_i}_{\hat{y}_i} + \epsilon$$

Least-squares regression

$$y_{i} = \underbrace{w_{0} + w_{1}x_{i}}_{\hat{y}_{i}} + \epsilon_{i}$$

• Find w_0 and w_1 , that minimize the prediction error:

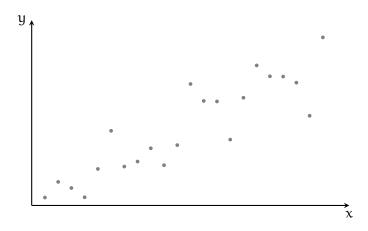
$$J(\boldsymbol{w}) = \sum_{i} \varepsilon_{i}^{2} = \sum_{i} (y_{i} - \hat{y}_{i})^{2} = \sum_{i} (y_{i} - (w_{0} + w_{1}x_{i}))^{2}$$

• We can minimize J(w) analytically

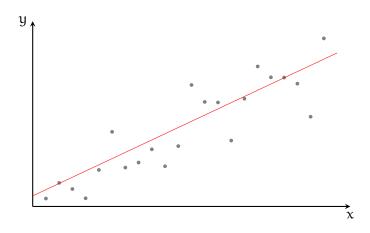
$$w_1 = r \frac{\mathrm{sd}_y}{\mathrm{sd}_x} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

^{*} See appendix for the derivation.

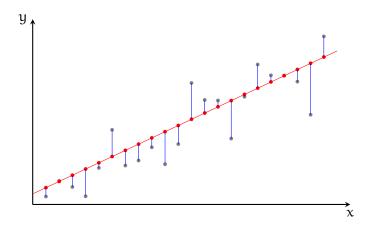
Visualization of least-squares regression



Visualization of least-squares regression



Visualization of least-squares regression



What is special about least-squares?

- Minimizing MSE (or SS_R) is equivalent to MLE estimate under the assumption $\varepsilon \sim \mathcal{N}(0,\sigma^2)$
- Working with 'minus log likelihood' is more convenient

$$J(w) = -\log \mathcal{L}(w) = -\log \prod_{i} \frac{e^{-\frac{(y_{i} - \hat{y}_{i})^{2}}{2\sigma^{2}}}}{\sigma\sqrt{2\pi}}$$

$$= \arg \min(-\log \mathcal{L}(w)) = \arg \min \sum_{i} (y_{i} - \hat{y}_{i})$$

$$\hat{\boldsymbol{w}} = \operatorname*{arg\,min}_{\boldsymbol{w}} (-\log \mathcal{L}(\boldsymbol{w})) = \operatorname*{arg\,min}_{\boldsymbol{w}} \sum_{i} (y_i - \hat{y}_i)^2$$

- There are other error functions, e.g., absolute value of the errors, that can be used (and used in practice)
- One can also estimate regression parameters using Bayesian estimation

Short digression: minimizing functions

In least squares regression, we want to find w_0 and w_1 values that minimize

$$J(w) = \sum_{i} (y_{i} - (w_{0} + w_{1}x_{i}))^{2}$$

- Note that J(w) is a *quadratic* function of $w = (w_0, w_1)$
- As a result, J(w) is *convex* and have a single extreme value
 there is a unique solution for our minimization problem
- In case of least squares regression, there is an analytic solution
- Even if we do not have an analytic solution, if our error function is convex, a search procedure like *gradient descent* can still find the *global minimum*

Measuring success in Regression

• *Root-mean-square error* (RMSE)

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

measures average error in the units compatible with the outcome variable.

Another well-known measure is the coefficient of determination

$$R^{2} = \frac{\sum_{i}^{n} (\hat{y}_{i} - \bar{y})^{2}}{\sum_{i}^{n} (y_{i} - \bar{y})^{2}} = 1 - \left(\frac{RMSE}{\sigma_{y}}\right)^{2}$$

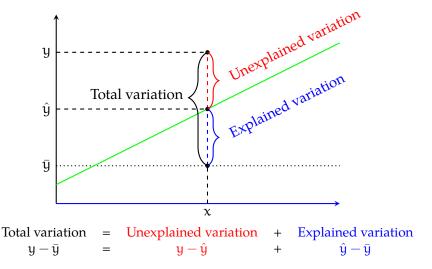
Assessing the model fit: r^2

We can express the variation explained by a regression model as:

$$\frac{\text{Explained variation}}{\text{Total variation}} = \frac{\sum_{i}^{n} (\hat{y}_{i} - \bar{y})^{2}}{\sum_{i}^{n} (y_{i} - \bar{y})^{2}}$$

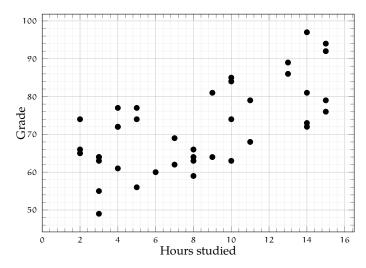
- This value is the square of the correlation coefficient
- The range of r^2 is [0, 1]
- $100 \times r^2$ is interpreted as 'the percentage of variance explained by the model'
- r^2 shows how well the model fits to the data: closer the data points to the regression line, higher the value of r^2

Explained variation



A hands-on exercise

Draw a regression line over the plot

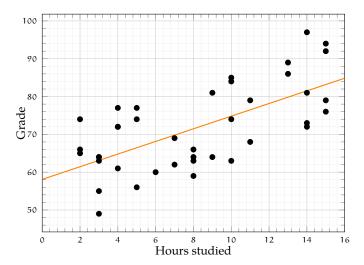


A hands-on exercise (cont.)

- What is the regression equation?
- What is the expected grade for a student who did did not study at all?
- What is the expected grade for a student who studied 12 hours?
- What is the expected grade for a student who studied 40 hours?

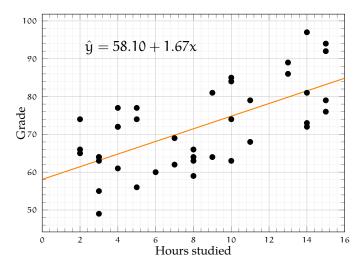
A hands-on exercise

The regression line



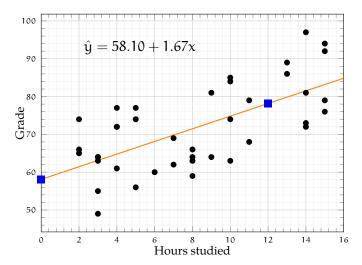
A hands-on exercise

The regression line



A hands-on exercise

The regression line



Regression with multiple predictors

$$y_{i} = \underbrace{w_{0} + w_{1}x_{i,1} + w_{2}x_{i,2} + \dots + w_{k}x_{i,k}}_{\hat{y}} + \epsilon_{i} = wx_{i} + \epsilon_{i}$$

 w_0 is the intercept (as before).

 $w_{1..k}$ are the coefficients of the respective predictors.

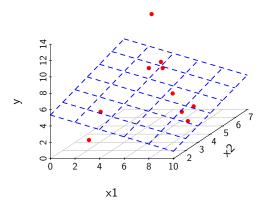
- ϵ is the error term (residual).
- using vector notation the equation becomes:

$$y_i = wx_i + \epsilon_i$$

where
$$w = (w_0, w_1, ..., w_k)$$
 and $x_i = (1, x_{i,1}, ..., x_{i,k})$

It is a generalization of simple regression with some additional power and complexity.

Visualizing regression with two predictors



Input/output of liner regression: some notation

A regression with k input variables and n instances can be described as:

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{y} = \underbrace{\begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,k} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,k} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & x_{n,2} & \dots & x_{n,k} \end{bmatrix}}_{X} \times \underbrace{\begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_k \end{bmatrix}}_{w} + \underbrace{\begin{bmatrix} \varepsilon_0 \\ \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix}}_{\varepsilon}$$

$$y = Xw + \epsilon$$

Estimation in multiple regression

$$y = Xw + \epsilon$$

We want to minimize the error (as a function of w):

$$\epsilon^2 = J(w) = (y - Xw)^2$$
$$= ||y - Xw||^2$$

Our least-squares estimate is:

$$\hat{\mathbf{w}} = \operatorname*{arg\,min}_{\mathbf{w}} \mathbf{J}(\mathbf{w})$$
$$= (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}}$$

Note: the least-squares estimate is also the maximum likelihood estimate under the assumption of normal distribution of errors.

Categorical predictors

- Categorical predictors are represented as multiple binary coded input variables
- For a binary predictor, we use a single binary input. For example, (1 for one of the values, and 0 for the other)

$$x = \begin{cases} 0 & \text{for male} \\ 1 & \text{for female} \end{cases}$$

• For a categorical predictor with k values, we use k-1 predictors (various coding schemes are possible). For example, for 3-values

$$\mathbf{x} = \begin{cases} (0,0,1) & \text{neutral} \\ (0,1,0) & \text{negative} \\ (1,0,0) & \text{positive} \end{cases} \quad \mathbf{x} = \begin{cases} (0,0) & \text{neutral} \\ (0,1) & \text{negative} \\ (1,0) & \text{positive} \end{cases}$$
one-hot coding 'treatment' encoding

Ç. Çöltekin, SfS / University of Tübingen

Dealing with non-linearity

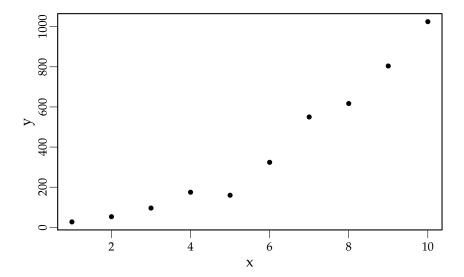
- Least squares works, because the loss function is linear with respect to parameter w
- Introducing non-linear combinations of inputs does not affect the estimation procedure. The following are still linear models

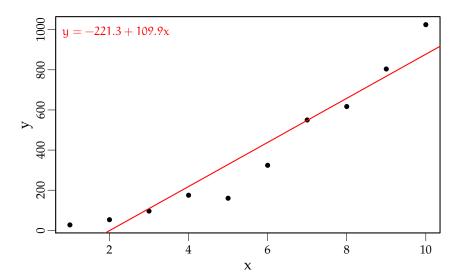
$$y_{i} = w_{0} + w_{1}x_{i}^{2} + \epsilon_{i}$$

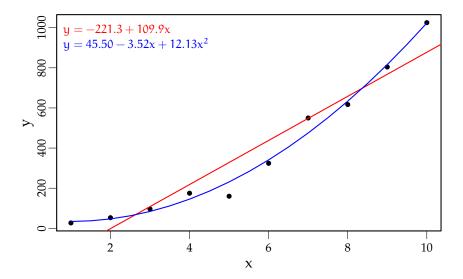
$$y_{i} = w_{0} + w_{1}\log(x_{i}) + \epsilon_{i}$$

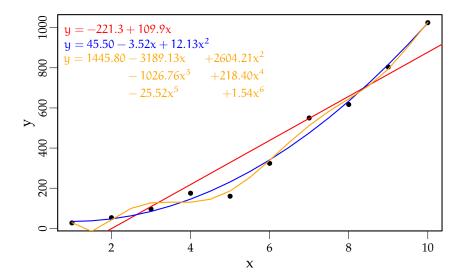
$$y_{i} = w_{0} + w_{1}x_{i,1} + w_{2}x_{i,2} + w_{3}x_{i,1}x_{i,2} + \epsilon_{i}$$

- These *transformations* allow linear models to deal with some non-linearities
- In general, we can replace input x by a function of the input(s) $\Phi(x)$. $\Phi(x)$ is called a *basis function*









Regularized parameter estimation

- To avoid overfitting and high variance, one of the common methods is regularization
- With regularization, in addition of minimizing the cost function, we simultaneously constrain the possible parameter values
- For example, the regression estimation becomes:

$$\hat{\mathbf{w}} = \operatorname*{arg\,min}_{w} \sum_{i} (y_{i} - \hat{y}_{i})^{2}$$

Regularized parameter estimation

- To avoid overfitting and high variance, one of the common methods is *regularization*
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- For example, the regression estimation becomes:

$$\hat{\mathbf{w}} = \operatorname*{arg\,min}_{\mathbf{w}} \sum_{\mathbf{i}} (\mathbf{y}_{\mathbf{i}} - \hat{\mathbf{y}}_{\mathbf{i}})^2 + \lambda \sum_{\mathbf{j}=1}^{k} w_{\mathbf{j}}^2$$

- The new part is called the regularization term, where λ is a *hyperparameter* that determines the effect of the regularization.
- In effect, we are preferring small values for the coefficients
- Note that we do not include w_0 in the regularization term

L2 regularization

The form of regularization, where we minimize the regularized cost function,

$$J(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|^2$$

is called L2 regularization.

- Note that we are minimizing the L2-norm of the weight vector
- In statistic literature this L2-regularized regression is called ridge regression
- The method is general: it can be applied to other ML methods as well
- The choice of λ is important
- Note that the scale of the input becomes important

L1 regularization

In L1 regularization we minimize

$$J(w) + \lambda \sum_{j=1}^{k} |w_j|$$

- The additional term is the L1-norm of the weight vector (excluding w₀)
- In statistic literature the L1-regularized regression is called *lasso*
- The main difference from L2 regularization is that L1 regularization forces some values to be 0 – the resulting model is said to be 'sparse'

Regularization as constrained optimization

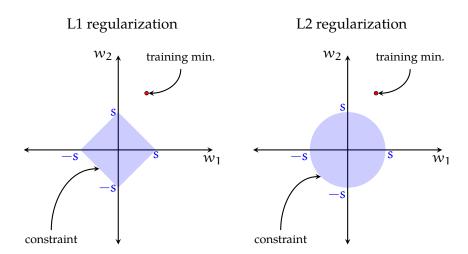
L1 and L2 regularization can be viewed as minimization with constraints

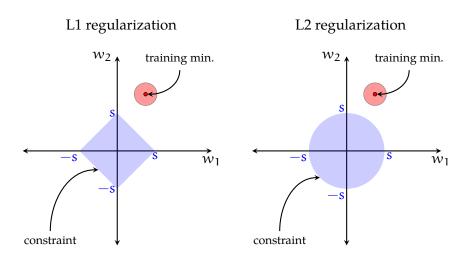
L2 regularization

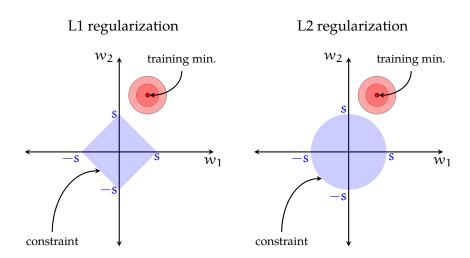
Minimize J(w) with constraint ||w|| < s

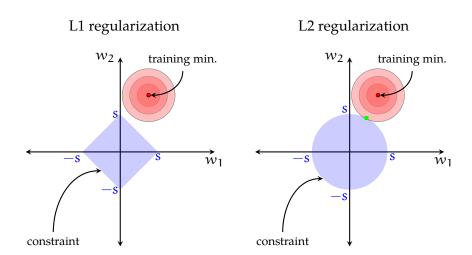
L1 regularization

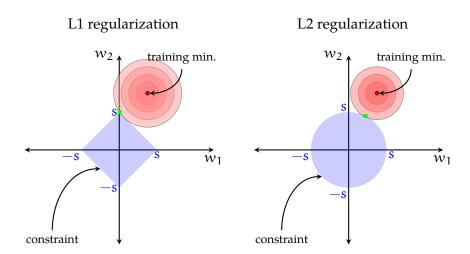
Minimize J(w) with constraint $||w||_1 < s$











Regularization: some remarks

- Regularization prevents overfitting and reduces variance
- The *hyperparameter* λ needs to be determined
 - best value is found typically using a grid search, or a random search
 - it is tuned on an additional partition of the data, development set
 - development set cannot overlap with training or test set
- The regularization terms can be interpreted as *priors* in a Bayesian setting
- Particularly, L2 regularization is equivalent to a normal prior with zero mean

Summary

What to remember:

- Supervised vs. unsupervised learning
- Regression vs. classification
- Linear regression equation
- Least-square estimate
- Next:

Mon classification

Wed exercises

Fri classification / ML evaluation

- MSE, r²
- non-linearity & basis functions
- L1 & L2 regularization (lasso and ridge)

Additional reading, references, credits

- Hastie, Tibshirani, and Friedman (2009) discuss introductory bits in chapter 1, and regression on chapter 3 (sections 3.2 and 3.4 are most relevant to this lecture)
- Jurafsky and Martin (2009) has a short section (6.6.1) on regression
- You can also consult any machine learning book (including the ones listed below)



Barber, David (2012). Bayesian Reasoning and Machine Learning. Cambridge University Press. 18BN: 9780521518147.



Hastie, Trevor, Robert Tibshirani, and Jerome Friedman (2009). The Elements of Statistical Learning: Data Mining, Inference, and Prediction. Second. Springer series in statistics. Springer-Verlag New York. ISBN: 9780387848587. URL: http://web.stanford.edu/-hastie/ElemStatLearn/.



James, G., D. Witten, T. Hastie, and R. Tibshirani (2013). An Introduction to Statistical Learning: with Applications in R. Springer Texts in Statistics. Springer New York. ISBN: 9781461471387. URL: http://www-bcf.usc.edu/-gareth/ISL/.

Additional reading, references, credits (cont.)



Jurafsky, Daniel and James H. Martin (2009). Speech and Language Processing: An Introduction to Natural Language Processing, Computational Linguistics, and Speech Recognition. second. Pearson Prentice Hall. ISBN: 978-0-13-504196-3.



Mitchell, Thomas (1997). Machine Learning. 1st. McGraw Hill Higher Education. ISBN: 0071154671,0070428077,9780071154673,9780070428072.