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University of Tübingen Seminar für Sprachwissenschaft

Summer Semester 2017

Machine learning is ...

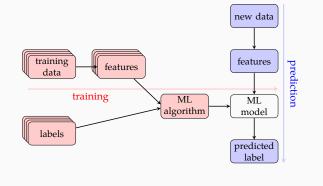
The field of machine learning is concerned with the question of how to construct computer programs that automatically improve with -Mitchell (1997) experience.

Machine Learning is the study of data-driven methods capable of mimicking, understanding and aiding human and biological information processing tasks. —Barber (2012)

Statistical learning refers to a vast set of tools for understanding data. —James et al. (2013)

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Supervised learning



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

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

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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.

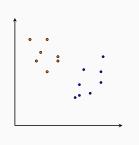
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Machine learning Regression

Unsupervised learning

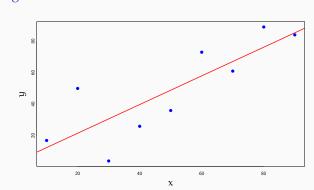
- In unsupervised learning we do not have any labels
- The aim is discovering some 'latent' structure in the data
- Common examples include
 - Clustering

 - Density estimationDimensionality reduction
- In NLP, methods that do not require (manual) annotation are sometimes called unsupervised



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Regression



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ML topics we will cover in this course

- (Linear) Regression (today)
- Classification / logistic regression (next week)

Machine learning Regression

- Evaluation ML methods / algorithms
- Unsupervised learning
- Neural networks / deep learning

Regression

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- 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
- · Sometimes, the border between the two is not clear

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Machine learning Regression

The simple linear model

$$y_i = a + bx_i + \varepsilon_i$$

- 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

- $\alpha + bx$ 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

Machine learning Regression

Estimating model parameters: reminder

In least-squares regression, we find

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

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

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

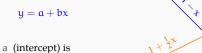
- take the derivative of J(w)
- set it to 0

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 $\bullet\,$ solve the resulting equation(s)

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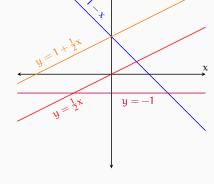
The linear equation: a reminder



b (slope) is the change in y as x is increased one unit.

where the line

crosses the y axis.



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Machine learning Regression

Notation differences for the regression equation

$$y_i = wx_i + \epsilon_i$$

- Sometimes, Greek letters α and β are used for intercept and the slope, respectively
- Another common notation to use only b, β , θ or w, but use subscripts, 0 indicating the intercept and 1 indicating the
- In machine learning it is common to use w for all coefficients (sometimes you may see b used instead of w_0)
- · 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 $\mathbf{x_i} = (1, x_i)$

Least-squares regression

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

• Find w_0 and w_2 , that minimize the prediction error:

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

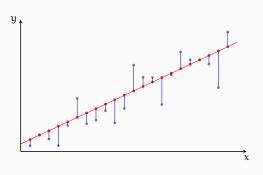
• We can minimize J(w) analytically

$$w_1 = r \frac{s d_y}{s d_x} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

* See appendix for the derivation

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Visualization of least-squares regression



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Machine learning Regression

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

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Machine learning Regression

Assessing the model fit: r^2

We can express the variation explained by a regression model

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

- 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'
- r² shows how well the model fits to the data: closer the data points to the regression line, higher the value of r²

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Machine learning Regression

Regression with multiple predictors

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

 w_0 is the intercept (as before).

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

- $\boldsymbol{\varepsilon}\$ 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.

What is special about least-squares?

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

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

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

- 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

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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

$$R^2 = \frac{\sum_i^n (\hat{y}_i - \bar{y})^2}{\sum_i^n (y_i - \bar{y})^2} = 1 - \left(\frac{RMSE}{\sigma_y}\right)^2$$

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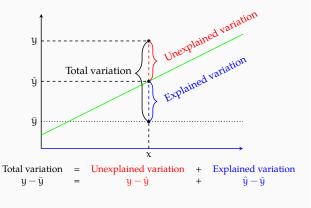
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Machine learning Regression

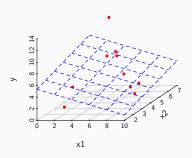
Explained variation

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Visualizing regression with two predictors



Input/output of liner regression: some notation

A regression with k input variables and n instances can be

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

 $y = Xw + \epsilon$

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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)

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

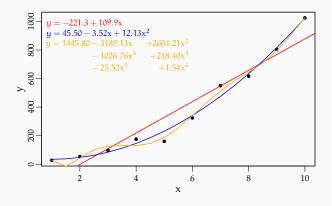
 $\bullet\,$ For a categorical predictor with k values, we use k-1predictors (various coding schemes are possible). For example, for 3-values

$$\mathbf{x} = \begin{cases} (0,0) & \text{for neutral} \\ (0,1) & \text{for negative} \\ (1,0) & \text{for positive} \end{cases}$$

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Example: polynomial basis functions



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L2 regularization

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

$$J(w) + \lambda ||w||$$

is called L2 regularization.

- · Note that we are minimizing the L2-norm of the weight
- 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

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:

$$\begin{split} \hat{\boldsymbol{w}} &= \operatorname*{arg\,min}_{\boldsymbol{w}} J(\boldsymbol{w}) \\ &= (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \end{split}$$

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

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

$$\begin{split} y_i &= w_0 + w_1 x_i^2 + \varepsilon_i \\ y_i &= w_0 + w_1 log(x_i) + \varepsilon_i \\ y_i &= w_0 + w_1 x_{i,1} + w_2 x_{i,2} + w_3 x_{i,1} x_{i,2} + \varepsilon_i \end{split}$$

- 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) $\Phi(x)$. $\Phi()$ is called a basis function

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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:

$$\hat{w} = \underset{w}{\arg\min} \sum_{i} (y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{k} w_j^2$$

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

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L1 regularization

In L1 regularization we minimize

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

- The additional term is the L1-norm of the weight vector (excluding w_0)
- In statistic literature the L1-regularized regression is called
- $\bullet\,$ The main difference from L2 regularization is that L1 regularization forces some values to be 0 - the resulting model is said to be 'sparse'

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L2 regularization

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

L1 regularization

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

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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
- · Particularly, L2 regularization is equivalent to a normal prior with zero mean

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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. ISBN: 9780521518147.

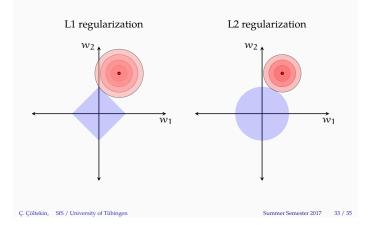
Hastie, Trevor, Robert Tibshirani, and Jerome Friedman (2009). The Elements of Statistical Learning: Data Mining, Inference, and Prediction. Second. Springer series in statistics. Springe URL: http://web.stanford.edu/-hastie/ElemStatLearn/.

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/.

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Visualization of regularization constraints



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Summary

What to remember:

- · Supervised vs. unsupervised learning
- Regression vs. classification • Linear regression equation
- Least-square estimate
- MSE, r²
- · non-linearity & basis functions
- L1 & L2 regularization

Next:

Wed n-gram language models (continued)

Fri exercises

Mon exercises (again)

Wed logistic regression

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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. 1888: 078-01-71-71-71-71-71-71-71



Mitchell, Thomas (1997). Machine Learning. 1st. McGraw Hill Higher Education. ISBN

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