Statistical Natural Language Processing ML intro & regression

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University of Tübingen Seminar für Sprachwissenschaft

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· Majority of the modern computational linguistic tasks and applications are based on machine learning

- Tokenization
- Part of speech tagging
- Parsing

Why machine learning?

- Speech recognition
- Named Entity recognition Document classification
- Question answering
- Machine translation

Supervised or unsupervised

Machine learning is ...

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

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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• Unsupervised methods try to find regularities in the data without any (direct) supervision

• Machine learning methods are often divided into two

• Supervised methods rely on labeled (or annotated) data

broad categories: supervised and unsupervised

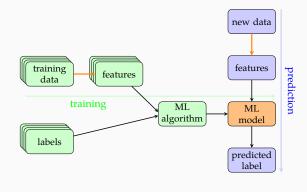
• Some methods do not fit any (or fit both):

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

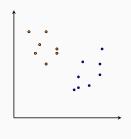


Unsupervised learning

• 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
- The methods that do not require (manual) annotation are sometimes called unsupervised



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Supervised learning

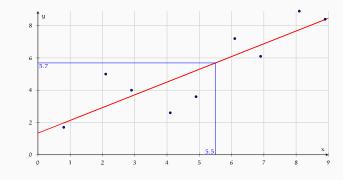
two common settings

A supervised ML method is called

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

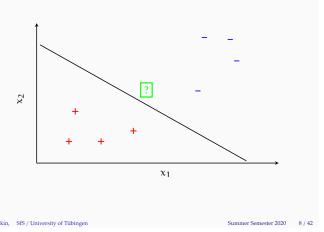
classification if the outcome to be predicted is a categorical variable

Regression



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Classification



Machine learning and statistics

- The methods largely overlap (it was even suggested that both should be collectively called 'data science')
- · Aims differ
 - In statistics (used as in experimental sciences) aim is making inferences using the models
 - In machine learning correct predictions are at the focus
- · A more diverse set of models/methods are used in ML

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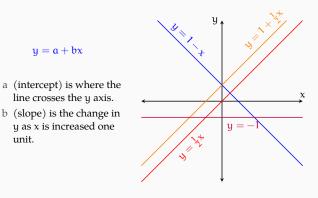
y = a + bx

line crosses the y axis.

y as x is increased one

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The linear equation: the regression model



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unit.

Notation differences for the regression equation

$$y_i = wx_i$$

- \bullet 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 $\mathbf{x_i} = (1, x_i)$

ML topics we will cover in this course

- (Linear) Regression (today)
- Classification (perceptron, logistic regression, ANNs)
- \bullet Evaluating ML methods / algorithms
- Unsupervised learning
- · Sequence learning

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Machine learning and models

- A machine learning method makes its predictions based
- The models are often parametrized: a set of parameters defines a model
- · Learning can be viewed as finding the 'best' model among a family of models (that differ based on their parameters)

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The simple linear model

some terminology

$$y_i = a + bx_i$$

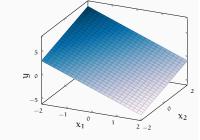
- y is the *outcome* (or response, or dependent) variable. The index i represents each unit observation/measurement (sometimes called a 'case')
- x is the *predictor* (or explanatory, or independent) variable
- a is the *intercept* (called *bias* in the NN literature)
- b is the slope of the regression line.

a and b are called coefficients or parameters

a + bx is the model's prediction of $y(\hat{y})$, given x

Regression models with multiple predictors

- The equation defines a (hyper)plane
- With 2 predictors: $y = w_0 + w_1 x_1 + w_2 x_2$
- With more predictors it is more convenient to use vector notation: y = wx



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Parameter estimation for regression

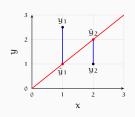
Parameter estimation

- In ML, we are interested in finding the best model based
- · Learning is selecting a model from a family of models that differ in their parameters
- Typically, we seek the parameters that reduce the prediction error on a training set
- Ultimately, we seek models that do not only do well on the training data, but also new, unseen instances

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Estimating regression parameters

- We view learning as a search for the regression equation with least error
- The error terms are also called residuals
- We want error to be low for the whole training set: average (or sum) of the error has to be reduced
- Can we minimize the sum of the errors?



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

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Short digression: minimizing functions

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

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

- Note that E(w) is a *quadratic* function of $w = (w_0, w_1)$
- As a result, E(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 the error function is convex, a search procedure like gradient descent can still find the global minimum

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Regression with multiple predictors

$$y_i = \underbrace{w_0 + w_1 x_{i,1} + w_2 x_{i,2} + \dots + w_k x_{i,k}}_{\hat{y}} + \varepsilon_i = w x_i + \varepsilon_i$$

 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
$$\mathbf{w} = (w_0, w_1, \dots, w_k)$$
 and $\mathbf{x_i} = \left(1, x_{i,1}, \dots, x_{i,k}\right)$

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

Least-squares regression

• Find w_0 and w_1 , that minimize the sum of the squared errors

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

ullet We can minimize $E(oldsymbol{w})$ analytically

$$w_1 = \frac{\sigma_{xy}}{\sigma_x^2} = r \frac{s d_y}{s d_x} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

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What is special about least-squares?

• Minimizing MSE (or SS_R) is equivalent to MLE estimate under the assumption $\varepsilon \sim \mathcal{N}(0,\sigma^2)$

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• Working with 'minus log likelihood' is more convenient

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

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

- 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

Evaluating machine learning systems

- Any (machine learning) system needs a way to measure its success
- For measuring success (or failure) in a machine learning system we need quantitative measures
- Remember that we need to measure the success outside the training data

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Measuring success in Regression

• Root-mean-square error (RMSE)

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i}^{n}(y_{i} - \hat{y}_{i})^{2}}$$

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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 In simple regression, it is the square of the correlation coefficient between the outcome and the predictor

We can express the variation explained by a regression model

Explained variation

Total variation

• The range of R^2 is [0,1]

Assessing the model fit: R²

as:

- * $100 \times R^2$ 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

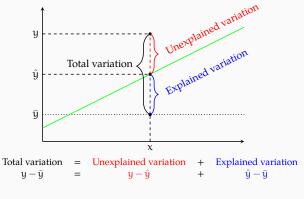
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Explained variation



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Dealing with non-linearity

- Least-squares estimation works because the regression equation is linear with respect to parameters \boldsymbol{w} (error function is quadratic)
- Introducing non-linear combinations of inputs does not affect the estimation procedure. The following are still linear models

$$y = w_0 + w_1 x^2 + \epsilon$$

$$y = w_0 + w_1 \log(x) + \epsilon$$

$$y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2 + \epsilon$$

- In general, we can replace input x by a function of the input(s) Φ(x). Φ() is called a basis function
- Basis functions allow linear models to model non-linear relations by transforming the input variables

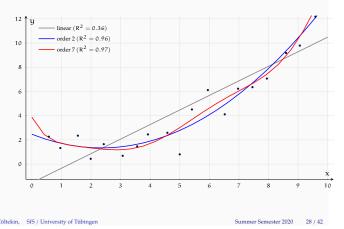
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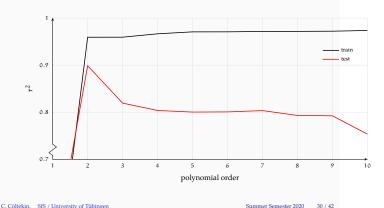
Example: polynomial basis functions



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Overfitting

demonstration through polynomial regression



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Overfitting

- Overfitting is an important problem in ML, happens when the model learns peculiarities/noise in the training data
- An overfitted model will perform well on training data, but worse on new/unseen data
- Typically 'more complex' models are more likely to overfit

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Preventing overfitting

- A straightforward approach is to chose a simpler model (family), e.g., by reducing the number of predictors
- More training data helps: it is less likely to overfit if number of training instances are (much) larger than the paramters
- There are other methods (one is coming on the next slide)
- We will return to this topic frequently during later lectures

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Regularized parameter estimation

- Regularization is a general method for avoiding overfitting
- The idea is to constrain the parameter values in addition to minimizing the training error
- For example, the regression estimation becomes:

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

- The new part is called the regularization term,
- \bullet λ is a *hyperparameter* that determines the strength 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

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 w_0)
- $\bullet\,$ In statistics 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'

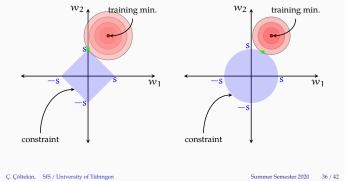
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L1 regularization

L2 regularization

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Visualization of regularization constraints



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Gradient descent for parameter estimation

- In many ML problems, we do not have a closed form solution for finding the minimum of the error function
- · In these cases, we use a search strategy
- Gradient descent is a search method for finding a minimum of a (error) function
- The general idea is to approach a minimum of the error function in small steps

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla \mathbf{J}(\mathbf{w})$$

 $\nabla J \;$ is the gradient of the loss function, it points to the direction of the maximum increase

 η is the learning rate

L2 regularization The form of regularization, where we minimize the regularized

$$J(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2$$

is called L2 regularization.

cost function,

- · Note that we are minimizing the L2-norm of the weight
- In statistic literature 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 also becomes important

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Regularization as constrained optimization

L1 and L2 regularization can be viewed as minimization with

L2 regularization

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

L1 regularization

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

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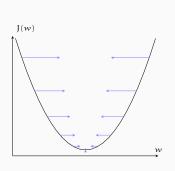
Regularization: some remarks

- · Regularization prevents overfitting
- 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

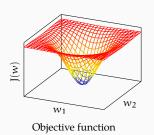
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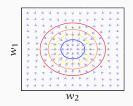
Gradient descent with single parameter

- · For a single parameter, gradient is a one-dimensional vector
- · The direction of gradient is towards the maximum increase
- · We take steps proportional to $-\nabla J(w)$
- · Steeper the curve, the larger the parameter update



Gradient descent with single parameter





Negative gradients

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 one-hot encoding (other coding schemes are possible)

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

Summary

What to remember:

- · Supervised vs. unsupervised learning
- Regression vs. classification
- · Linear regression equation
- Least-square estimate
- MSE, R²
- non-linearity & basis functions
- (lasso and ridge)

Next:

Wed,Fri classification

Mon ML evaluation

- L1 & L2 regularization

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)







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. sasc. 978-01-35-0319-63.

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Additional reading, references, credits (cont.)

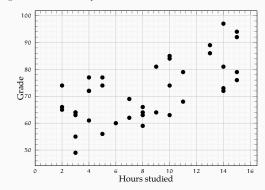


Mitchell, Thomas (1997). Machine Learning. 1st. McGraw Hill Higher Education. 1st

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A hands-on exercise

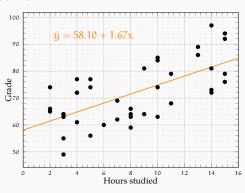
Draw a regression line over the plot



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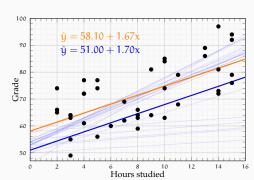
A hands-on exercise

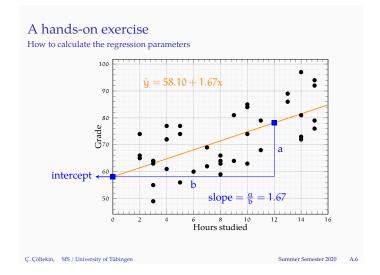
The regression line

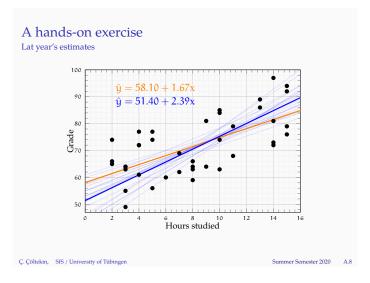


A hands-on exercise

Your estimates

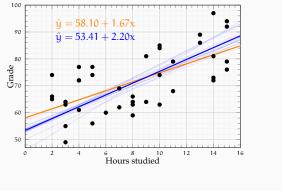






A hands-on exercise

Your estimates (some removed)



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