Statistical Natural Language Processing

ML intro & regression

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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. —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)

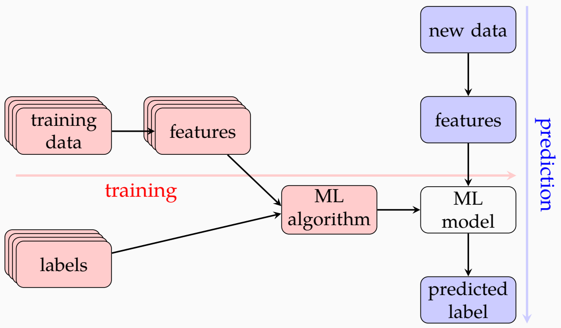
Statistical learning refers to a vast set of tools for understanding data. —James et al. (2013)

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

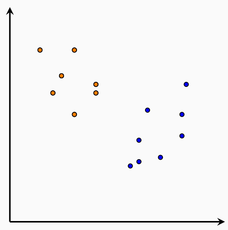
In this course, we will mostly discuss/use supervised methods.

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



Supervised learning

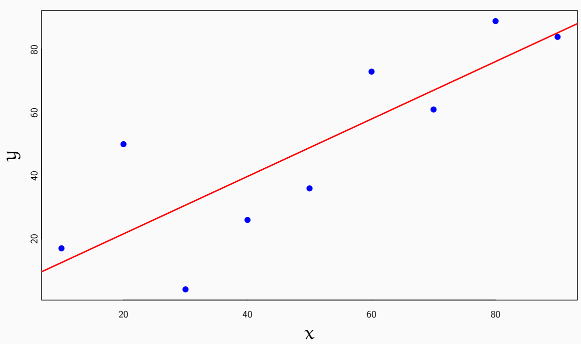
two common settings

An ML algorithm is called

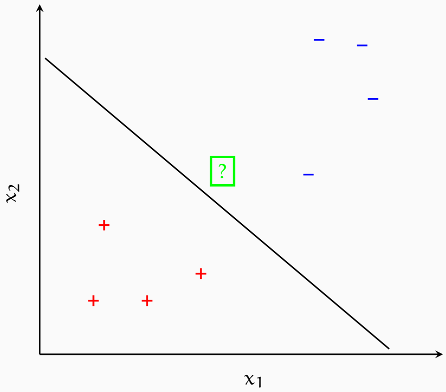
regression if the outcome to be predicted is a numeric (continuous) variable

classification if the outcome to be predicted is a categorical variable

Regression



Classification



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

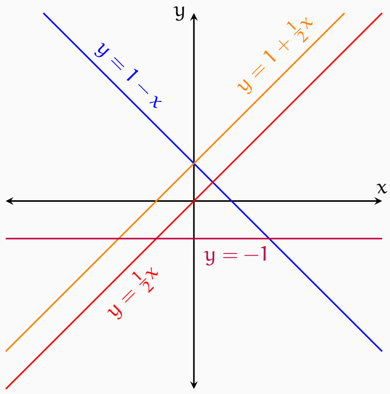
- Regression is a (supervised) method for predicting the value of a continuous response variable based on a number of predictors
- We estimate the conditional expectation of the outcome variable given the predictor(s)
- It is the foundation of many models in statistics and machine learning
- If the outcome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

Notation differences for the regression equation

$$y_i = \boldsymbol{w}\boldsymbol{x}_i + \epsilon_i$$

- 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 slope
- 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: $\boldsymbol{w} = (w_0, w_1)$ and $\boldsymbol{x}_i = (1, x_i)$

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 $J(\boldsymbol{w})$ (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 $J(\boldsymbol{w})$
- set it to 0
- solve the resulting equation(s)

Least-squares regression

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

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

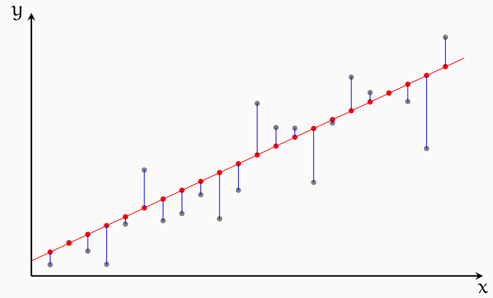
$$J(\boldsymbol{w}) = \sum_i \epsilon_i^2 = \sum_i (y_i - \hat{y}_i)^2 = \sum_i (y_i - (w_0 + w_1 x_i))^2$$

- We can minimize $J(\boldsymbol{w})$ analytically

$$w_1 = r\frac{sd_x}{sd_y} \qquad w_0 = \bar{y} - w_1\bar{x}$$

* See appendix for the derivation.

Visualization of least-squares regression



What is special about least-squares?

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

$$J(\boldsymbol{w}) = -\log \mathcal{L}(\boldsymbol{w}) = -\log \prod_i \frac{e^{-\frac{(y_i - \hat{y}_i)^2}{2\sigma^2}}}{\sigma\sqrt{2\pi}}$$

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}}(-\log \mathcal{L}(\boldsymbol{w})) = \arg\min_{\boldsymbol{w}} \sum_i (y_i - \hat{y}_i)^2$$

- 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

$$J(\boldsymbol{w}) = \sum_i (y_i - (w_0 + w_1 x_i))^2$$

- Note that $J(\boldsymbol{w})$ is a *quadratic* function of $\boldsymbol{w} = (w_0, w_1)$
- As a result, $J(\boldsymbol{w})$ 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)

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

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

- Another well-known measure is the *coefficient of determination*

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

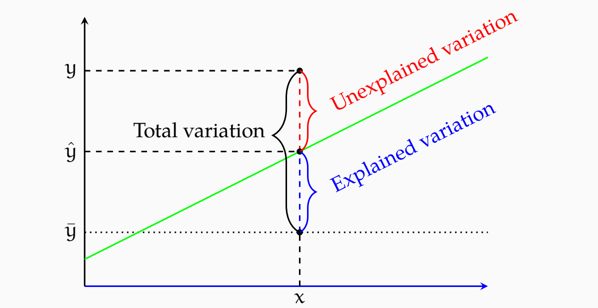
Assessing the model fit: r^2

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

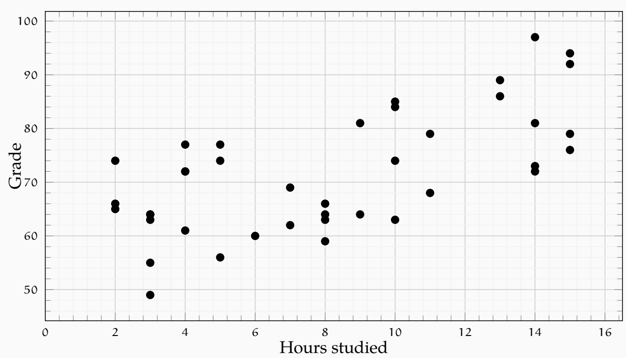
Explained variation



Total variation	=	Unexplained variation	+	Explained variation
$y - \bar{y}$	=	$y - \hat{y}$	+	$\hat{y} - \bar{y}$

A hands-on exercise

Draw a regression line over the plot

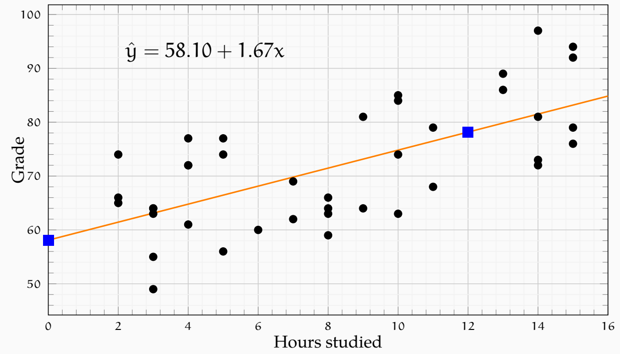


A hands-on exercise (cont.)

- 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



Regression with multiple predictors

$$y_i = \underbrace{w_0 + w_1 x_{i,1} + w_2 x_{i,2} + \ldots + w_k x_{i,k}}_{\hat{y}} + \epsilon_i = \boldsymbol{w}\boldsymbol{x}_i + \epsilon_i$$

w_0 is the intercept (as before).

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

ϵ is the error term (residual).

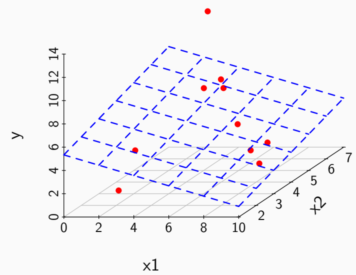
- using vector notation the equation becomes:

$$y_i = \boldsymbol{w}\boldsymbol{x}_i + \epsilon_i$$

where $\boldsymbol{w} = (w_0, w_1, \ldots, w_k)$ and $\boldsymbol{x}_i = (1, x_{i,1}, \ldots, x_{i,k})$

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:

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{\boldsymbol{y}} = \underbrace{\begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \ldots & x_{1,k} \\ 1 & x_{2,1} & x_{2,2} & \ldots & x_{2,k} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & x_{n,2} & \ldots & x_{n,k} \end{bmatrix}}_{\mathbf{X}} \times \underbrace{\begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_k \end{bmatrix}}_{\boldsymbol{w}} + \underbrace{\begin{bmatrix} \epsilon_0 \\ \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}}_{\boldsymbol{\epsilon}}$$

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{w} + \boldsymbol{\epsilon}$$

Estimation in multiple regression

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{w} + \boldsymbol{\epsilon}$$

We want to minimize the error (as a function of $\boldsymbol{w}$):

$$\begin{aligned} \boldsymbol{\epsilon}^2 = J(\boldsymbol{w}) &= (\boldsymbol{y} - \mathbf{X}\boldsymbol{w})^2 \\ &= \|\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\|^2 \end{aligned}$$

Our least-squares estimate is:

$$\begin{aligned} \hat{\boldsymbol{w}} &= \arg\min_{\boldsymbol{w}} J(\boldsymbol{w}) \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \end{aligned}$$

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

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

one-hot coding 'treatment' encoding

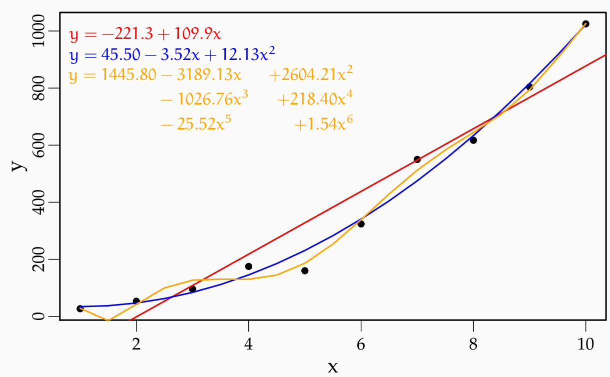
Dealing with non-linearity

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

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

- 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*

Example: polynomial basis functions



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:

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

- The new part is called the regularization term, 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,

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

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

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

- The additional term is the L1-norm of the weight vector (excluding w_0)
- 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

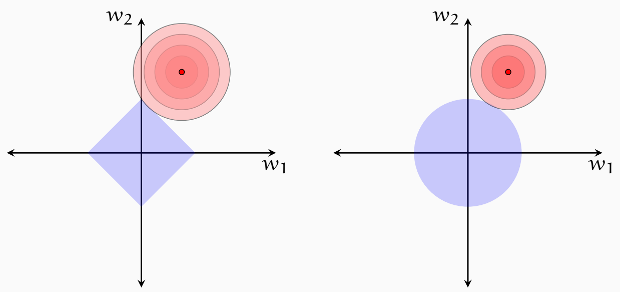
$$\text{Minimize} \quad J(w) \quad \text{with constraint} \quad \|\boldsymbol{w}\| < s$$

L1 regularization

$$\text{Minimize} \quad J(w) \quad \text{with constraint} \quad \|\boldsymbol{w}\|_1 < s$$

Visualization of regularization constraints

L1 regularization L2 regularization



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
- MSE, r^2
- non-linearity & basis functions
- L1 & L2 regularization (lasso and ridge)

Next:

Mon classification
Wed exercises
Fri classification / ML evaluation

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. 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.