Introduction to ML and Regression

Statistical Natural Language Processing

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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)

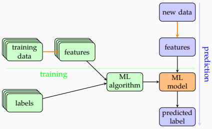
Statistical learning refers to a vast set of tools for understanding data. —James et al. (2013)

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

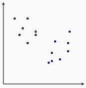
In this course, we will mostly discuss/use supervised methods.

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



Supervised learning

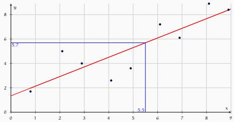
two common settings

A supervised ML method is called

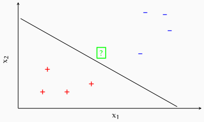
regression if the outcome to be predicted is a numeric (continuous) variable

classification if the outcome to be predicted is a categorical variable

Regression



Classification



ML topics we will cover in this course

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

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

Machine learning and models

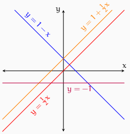
- A machine learning method makes its predictions based on a model
- The models are often parametrized: a set of parameters defines a model
- Learning can be viewed as finding the 'best' model among a family of models (that differ based on their parameters)

The linear equation: the regression model

$$y = a + bx$$

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

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

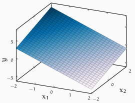
Notation differences for the regression equation

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

- 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 $\boldsymbol{x}_i = (1, x_i)$

Regression models with multiple predictors

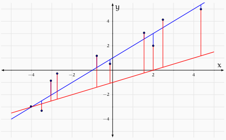
- The equation defines a (hyper)plane
- With 2 predictors: $y = w_0 + w_1x_1 + w_2x_2$
- With more predictors it is more convenient to use the vector notation: $y = \boldsymbol{w}\boldsymbol{x}$



Parameter estimation

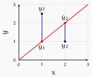
- In ML, we are interested in finding the best model based on data
- Learning is selecting a model from a family of models that differ in their parameters
- Typically, we seek the parameters that reduce the prediction error on a training set
- Ultimately, we seek models that do not only do well on the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

Parameter estimation for regression



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?



$$y_i = \underbrace{w_0 + w_1x_i}_{\hat{y}_i} + \epsilon_i$$

Least-squares regression

- Find w_0 and w_1, that minimize the *sum of the squared errors* (SSE)

$$E(\boldsymbol{w}) = \sum_i \epsilon_i^2 = \sum_i (y_i - \hat{y}_i)^2 = \sum_i (y_i - (w_0 + w_1x_i))^2$$

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

$$w_1 = \frac{\sigma_{xy}}{\sigma_x^2} = r\frac{sd_y}{sd_x} \qquad w_0 = \bar{y} - w_1\bar{x}$$

Short digression: minimizing functions

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

$$E(\boldsymbol{w}) = \sum_i (y_i - (w_0 + w_1x_i))^2$$

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

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

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

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

- 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

Regression with multiple predictors

$$y_i = \underbrace{w_0 + w_1x_{i,1} + w_2x_{i,2} + \ldots + w_kx_{i,k}}_{\hat{y}} + \epsilon_i = \boldsymbol{w}\boldsymbol{x}_i + \epsilon_i$$

- w_0 is the intercept (as before).
- $w_{1..k}$ are the coefficients of the respective predictors.
- ϵ is the error term (residual).
- using the 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.

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

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*

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

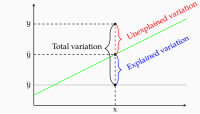
Assessing the model fit: R^2

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

$$\frac{\text{Explained variation}}{\text{Total variation}} = \frac{\sum_i^n(\hat{y}_i - \bar{y})^2}{\sum_i^n(y_i - \bar{y})^2}$$

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

$y - \bar{y} = y - \hat{y} + \hat{y} - \bar{y}$

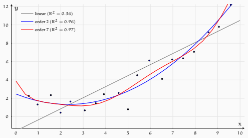
Dealing with non-linearity

- 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) $\Phi(x)$. $\Phi()$ is called a *basis function*
- Basis functions allow linear models to model non-linear relations by *transforming* the input variables

Example: polynomial basis functions

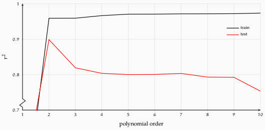


Overfitting

- *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

Overfitting

demonstration through polynomial regression



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

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:

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

- The new part is called the regularization term,
- 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

L2 regularization

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

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

is called L2 regularization.

- Note that we are minimizing the L2-norm of the weight vector
- In statistic literature 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

L1 regularization

In L1 regularization we minimize

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

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

Regularization as constrained optimization

L1 and L2 regularization can be viewed as minimization with constraints

L2 regularization

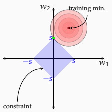
Minimize $E(w)$ with constraint $\|\boldsymbol{w}\| < s$

L1 regularization

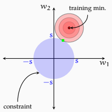
Minimize $E(w)$ with constraint $\|\boldsymbol{w}\|_1 < s$

Visualization of regularization constraints

L1 regularization



L2 regularization



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

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

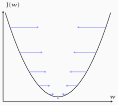
$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla J(\boldsymbol{w})$$

∇J is the gradient of the loss function, it points to the direction of the maximum increase

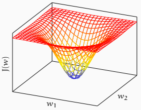
η is the learning rate

Gradient descent with single parameter

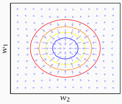
- For a single parameter, gradient is a one-dimensional vector
- The direction of gradient is towards the maximum increase
- We take steps proportional to $-\nabla J(w)$
- Steeper the curve, the larger the parameter update



Gradient descent with single parameter



Objective function



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)

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

Summary

What to remember:

- Supervised vs. unsupervised learning
- Regression vs. classification
- Linear regression equation
- Least-square estimate
- MSE, R^2
- non-linearity & basis functions
- L1 & L2 regularization (lasso and ridge)

Next:

Wed classification

Fri first lab session

Mon classification

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/`.

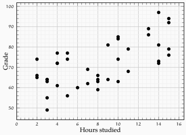
James, G., D. Witten, T. Hastie, and R. Tibshirani (2013). *An Introduction to Statistical Learning: with Applications in R*. Springer Texts in Statistics. Springer New York. ISBN: 9781461471387. URL: `http://www-bcf.usc.edu/~gareth/ISL/`.

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.

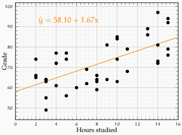
A hands-on exercise

Draw a regression line over the plot



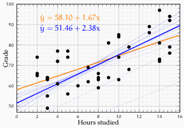
A hands-on exercise

The regression line



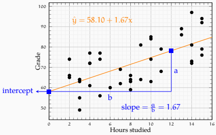
A hands-on exercise

Your estimates



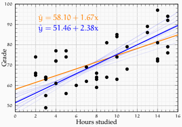
A hands-on exercise

How to calculate the regression parameters



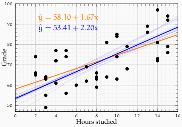
A hands-on exercise

Your estimates (some removed)



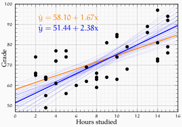
A hands-on exercise

Estimates from 2020



A hands-on exercise

Regression estimates 2019–2021



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