Martin Mundt, Dr. Iuliia Pliushch, Prof. Dr. Visvanathan Ramesh

Pattern Analysis & Machine Intelligence
Praktikum: MLPR-19

Week 2: Regression and Gradient Descent

Reminder: Lecture requirements

- 4 hours per week
- 8 credit points
- Final class group projects
- Attend the class

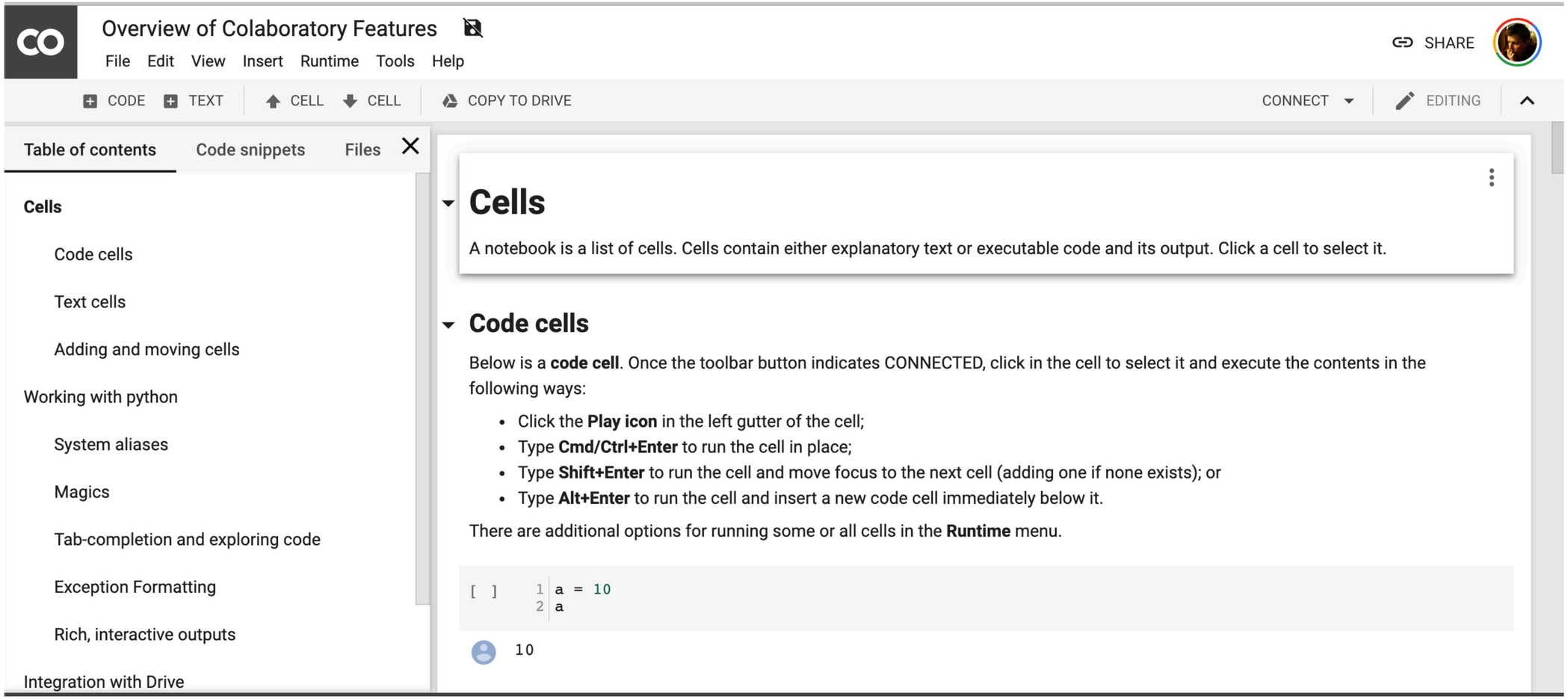
- Bring a laptop
- Each session is going to start with a small lecture
- Jupyter notebooks will be used for practical content
- We will use Google's Collaboratory for cloud computation
- If you want to execute the notebooks locally, we advise a Linux or Mac OS

- Lecture materials will be shared on GitHub: https://github.com/MrtnMndt/mlpr19

Reminder: Tentative schedule

Week 1: 15.04 – Intro Jupyter & Colab notebooks, Python review, version-control & documentation
22.04 – Easter holiday
Week 2: 29.04 – Regression and gradient descent (Kaggle Titanic dataset)
Week 3: 06.05 – Random forests (Sklearn intro & San Francisco Crime Challenge)
Week 4: 13.05 – Intro to unsupervised learning (K-means or PCA)
Week 5: 20.05 – Basic neural networks (Multi-layer perceptron on FashionMNIST)
Week 6: 27.05 – Convolutional neural networks & frameworks (PyTorch, Revisiting FashionMNIST)
Week 7: 03.06 – Unsupervised NNs (autoencoders, image generation - variational autoencoders)
10.06 – Pfingsten
Week 8: 17.06 – Intro to basic reinforcement learning (Cart-pole)
Week 9: 24.06 – Reinforcement learning: Q-Learning and QNN (some game)
Week 10: 01.07 – Neural sequence models (Recurrent neural networks, text classification)
Week 11: 08.07 – Neural sequence models (long-short-term memory, poetry generation)
Week 12: 15.07 – State of the art outlook, project pitches and discussion (3 slide pitches)

Reminder: Google Colab: https://colab.research.google.com/



Machine Learning

Supervised: Target outputs (labelled) are known and can be used for training

* Regression, Classification

Unsupervised: Target outputs not defined or unavailable

* Density estimation, clustering

Linear Regression

- Expresses a linear relationship between several independent **x** and a dependent variable **y** (labeled target)

$$t = w_0 + \sum_{i=1}^{D} w_i x_i + \varepsilon$$

- Regression weights **w** are parameters of the model linking inputs **x** with targets **t**

- In machine learning terminology linear regression is a supervised learning algorithm with continuous targets, i.e. it assumes a labeled dataset **D** with N training pairs of inputs and targets.

Linear Regression: how do we find the model weights?

- Need a way to measure the performance of the linear model with different weights

$$MSE_D(w) = \frac{1}{2}\sum_{n=1}^{N}(w_0 + \sum_i w_i x_{ni} - t_n)^2$$

- In ML this is referred to as a cost function and it measures the error of the model with respect to the weights **w**. (In this case the mean-squared difference between prediction and target)

- The optimal regression weights can be found by minimizing this error

$$w_{LR} = argmin_w MSE_D(w) = argmin_w \frac{1}{2}\sum_{n=1}^{N}(w_0 + \sum_i w_i x_{ni} - t_n)^2$$

Solving linear regression

- We can express linear regression in matrix notation if we extend $x_0 \equiv 1$ and denote the transposed weight vector as $\boldsymbol{w}^T$

$$t = \boldsymbol{w}^T \boldsymbol{x} + \varepsilon$$

- The minimization problem can then be written as

$$w_{LR} = argmin_w \frac{1}{2} \sum_{n=1}^{N} (t_n - \boldsymbol{w}^T \boldsymbol{x}_n)^2$$

Solving linear regression

- We can solve this analytically

$$\frac{\partial}{\partial w_i}\frac{1}{2}\sum_{n=1}^{N}(t_n - \boldsymbol{w}^T\boldsymbol{x}_n)^2 = \sum_{n=1}^{N}(t_n - \boldsymbol{w}^T\boldsymbol{x}_n)x_{in} = 0 \;\; \forall\, i$$

$$\Rightarrow \boldsymbol{w}_{LR}^T\left(\sum_{n=1}^{N}\boldsymbol{x}_n\boldsymbol{x}_n^T\right) = \sum_{i=1}^{N}t_n\boldsymbol{x}_n^T$$

- If we collect all training samples into a matrix $\boldsymbol{X} = (\boldsymbol{x}_1^T, \dots, \boldsymbol{x}_N^T) \in \mathbb{R}^{N\times(D+1)}$ and a target vector $\boldsymbol{t} = (t_1, \dots, t_N)^T$, we can write the optimal regression weights as

$$\boldsymbol{w}_{LR} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{t}$$

Linear regression in practice

- Let's take a look at practical linear regression in

https://github.com/PyMLVizard/PyMLViz

- PyMLViz is a project together with Prof. Dr. Bertschinger that features interactive widgets to explore different basic machine learning algorithms inside the browser.

- We can extend linear regression to more complicated basis functions, e.g. polynomial or radial basis functions. This is further explained in the notebook we will go through.

- If you haven't been able to attend the practice please take a look at the linear regression notebook at above URL, including polynomial and radial basis functions.

Logistic Regression

- Actually a technique for classification, i.e. $Y = \{0, 1\}$, with a probabilistic viewpoint.
- Goal is to correctly classify input x into one of two classes
- We could technically also do classification with the linear regression model we have just learned and treat the output as class 1 if the prediction surpasses a threshold and class 0 otherwise.
- In logistic regression we would like to interpret our model's decisions based on class probabilities $P(y = 1|x)$

Logistic Regression

- For binary classification we can write decisions based on the log odds.
  * If neither outcome is favored => log odds = 0
  * If one outcome is favored by log odds = x, the other is disfavored with –x

- We learn the log odds of P(y = 1|x) as a linear function:

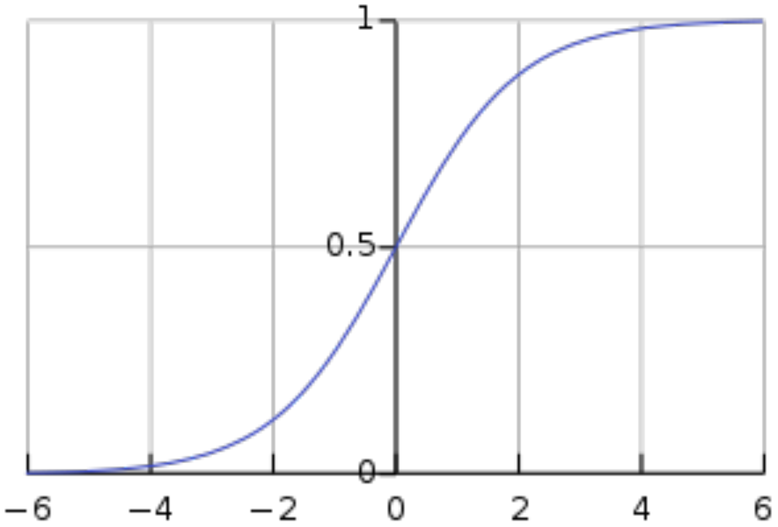
$$\log \frac{P(y=1|\boldsymbol{x})}{P(y=0|\boldsymbol{x})} = w_0 + \boldsymbol{x}^T \boldsymbol{w}_1$$

- Probabilities <-> log odds

$$z = log \frac{p}{1-p} \qquad e^z = \frac{p}{1-p} \qquad p = \frac{1}{1+e^{-z}} \; (logistic\ function)$$

Logistic Regression

$$\Rightarrow P(y = 1|\boldsymbol{x}, \boldsymbol{w}) = \frac{1}{1 + e^{-(w_0 + \boldsymbol{x}^T \boldsymbol{w}_1)}}$$



https://en.wikipedia.org/wiki/Sigmoid_function

- Again, we can find the maximum log likelihood by setting the derivatives of the log-likelihood with respect to the weights (parameters) to zero

$$\frac{\partial}{\partial w_i} \frac{1}{N} \sum_{n=1}^{N} [y_n \log\big(P(y_n = 1|x_n, w) + (1 - y_n) \log\big(1 - P(y_n = 1|x_n, w)\big)\big] = 0$$

- We need to derive above expression (apply the chain rule multiple times). Because above expression isn't closed form we have to solve it numerically by maximizing the likelihood or using e.g. gradient descent to minimize the negative thereof. This cost function is typically referred to as the Cross Entropy loss.

Logistic Regression cost function derivation

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{\partial}{\partial \theta_j} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log\left(h_\theta\left(x^{(i)}\right)\right) + (1 - y^{(i)}) \log\left(1 - h_\theta\left(x^{(i)}\right)\right) \right]$$

$$\underset{\text{linearity}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\partial}{\partial \theta_j} \log\left(h_\theta\left(x^{(i)}\right)\right) + (1 - y^{(i)}) \frac{\partial}{\partial \theta_j} \log\left(1 - h_\theta\left(x^{(i)}\right)\right) \right]$$

$$\underset{\text{chain rule}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\frac{\partial}{\partial \theta_j} h_\theta\left(x^{(i)}\right)}{h_\theta\left(x^{(i)}\right)} + (1 - y^{(i)}) \frac{\frac{\partial}{\partial \theta_j}\left(1 - h_\theta\left(x^{(i)}\right)\right)}{1 - h_\theta\left(x^{(i)}\right)} \right]$$

$$\underset{h_\theta(x) = \sigma\left(\theta^\top x\right)}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\frac{\partial}{\partial \theta_j} \sigma\left(\theta^\top x^{(i)}\right)}{h_\theta\left(x^{(i)}\right)} + (1 - y^{(i)}) \frac{\frac{\partial}{\partial \theta_j}\left(1 - \sigma\left(\theta^\top x^{(i)}\right)\right)}{1 - h_\theta\left(x^{(i)}\right)} \right]$$

$$\underset{\sigma'}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{\sigma\left(\theta^\top x^{(i)}\right)\left(1 - \sigma\left(\theta^\top x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{h_\theta\left(x^{(i)}\right)} - (1 - y^{(i)}) \frac{\sigma\left(\theta^\top x^{(i)}\right)\left(1 - \sigma\left(\theta^\top x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{1 - h_\theta\left(x^{(i)}\right)} \right]$$

$$\underset{\sigma\left(\theta^\top x\right) = h_\theta(x)}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \frac{h_\theta\left(x^{(i)}\right)\left(1 - h_\theta\left(x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{h_\theta\left(x^{(i)}\right)} - (1 - y^{(i)}) \frac{h_\theta\left(x^{(i)}\right)\left(1 - h_\theta\left(x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{1 - h_\theta\left(x^{(i)}\right)} \right]$$

$$\underset{\frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right) = x_j^{(i)}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} \left(1 - h_\theta\left(x^{(i)}\right)\right) x_j^{(i)} - \left(1 - y^{i}\right) h_\theta\left(x^{(i)}\right) x_j^{(i)} \right]$$

$$\underset{\text{distribute}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{i} - y^{i} h_\theta\left(x^{(i)}\right) - h_\theta\left(x^{(i)}\right) + y^{(i)} h_\theta\left(x^{(i)}\right) \right] x_j^{(i)}$$

$$\underset{\text{cancel}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[y^{(i)} - h_\theta\left(x^{(i)}\right) \right] x_j^{(i)}$$

$$= \frac{1}{m} \sum_{i=1}^{m} \left[h_\theta\left(x^{(i)}\right) - y^{(i)} \right] x_j^{(i)}$$

$$\frac{d}{dx}\sigma(x) = \frac{d}{dx}\left(\frac{1}{1 + e^{-x}}\right)$$

$$= \frac{-(1 + e^{-x})'}{(1 + e^{-x})^2}$$

$$= \frac{e^{-x}}{(1 + e^{-x})^2}$$

$$= \left(\frac{1}{1 + e^{-x}}\right)\left(\frac{e^{-x}}{1 + e^{-x}}\right)$$

$$= \left(\frac{1}{1 + e^{-x}}\right)\left(\frac{1 + e^{-x}}{1 + e^{-x}} - \frac{1}{1 + e^{-x}}\right)$$

$$= \sigma(x)\left(\frac{1 + e^{-x}}{1 + e^{-x}} - \sigma(x)\right)$$

$$= \sigma(x)\left(1 - \sigma(x)\right)$$

Taken from:

https://stats.stackexchange.com/questions/278771/how-is-the-cost-function-from-logistic-regression-derivated

Logistic Regression and Gradient Descent

- Let's **solve our logistic regression with gradient descent.** In fact this will be useful because what we have just seen and will learn about gradient descent, will be our first building block when we go on to e.g. neural networks later.

- What is gradient descent?
  * In its simplest form, it is a first order optimization algorithm designed to find the minimum of a differentiable function.
  * This is achieved by iteratively taking (small) steps towards the negative of the gradient. For a function f($\mathbf{x}$) this is the direction in which it decreases the fastest.

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - \lambda \nabla f(\boldsymbol{x}_n)$$

- With a step size lambda (called learning rate in ML) we can find the minimum of the function such that

$$f(\boldsymbol{x}_0) \geq f(\boldsymbol{x}_1) \geq \ \ldots \ \geq f(\boldsymbol{x}_n)$$

Gradient Descent: the ML perspective

- The previous slide gave a definition of how to apply gradient descent to a function. How do we use gradient descent for ML?
  => We calculate the gradient based on the cost/loss function and our model's predictions and iteratively learn a good set of parameters θ (in ML we generally optimize θ as there can be many more parameters than just the weights)

- We have already seen two such loss functions $\mathcal{L}$ that we can numerically optimize: the MSE and Cross-Entropy loss functions.

- In the simplest form we can directly update our weights with the calculated gradients

$$\theta = \theta - \lambda \nabla \mathcal{L}(\theta) = \theta - \lambda \frac{1}{N} \sum_{n=1}^{N} \nabla \mathcal{L}_n(\theta)$$

Gradient Descent

- We will use gradient descent in this week's notebook to optimize a logistic regression on the Titanic passenger dataset.

- Before we proceed: gradient descent doesn't come without caveats and thus there is many variants of gradient descent that address individual aspects, including stochastic update rules or adaptive learning rates. We will again take a look at some interactive widgets in:

https://github.com/PyMLVizard/PyMLViz

- If you haven't been able to attend the lectures you should read and explore the articles on introduction to gradient descent and the follow-up on its variants (SGD, momentum, nesterov, AdaGrad, Adam etc.)