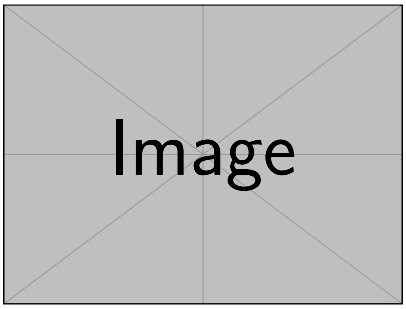
Autumn semester 2025



Data-Mining in Environmental Science

Learning diary

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Contents

1. Orientation

My personal background is that I am an exchange student in physics, studying at the University of Eastern Finland for the autumn semester. As such I have quite a strong background in programming, especially in Python, statistics and machine learning already. As I am quite interested in these topics and my home university offers a rather flexible study plan, I further deepened my knowledge by choosing multiple electives and a Bachelor thesis topic that were deeply connected with data analysis already. Although I expect that many things in the beginning of the course will be topics I already learned, I am very much looking forward to developing a deeper understanding of Data mining and seeing this done in a context I have no previous knowledge yet – namely Environmental science. Looking at the curriculum, there are also many topics I have had no prior experience in which is quite exciting to me. In summary, I expect this course to build nicely on my previous knowledge while additionally providing interesting insights to the field of Environmental science.

As a physics student, I am very used to writing scientific paper-like reports. This is the idea behind many reports of practicals I already needed to write as well as my Bachelor thesis. In these the expression of ones own opinion is actively discouraged. I would even go further and say that conciseness and scientific correctness are virtues hammered into us for years during our studies. Naturally a Learning diary such as this where the expression of a personal opinion and a critical reflection about the topics learned is not only encouraged but actively required is therefore quite a step out of my comfort zone. Still, I am looking forward to experiencing this new concept and seeing how it will shape my learning experience. At least at the time of starting this course this integrated approach of always putting learned things in ones own context, thinking critically and still performing quantitative task during the exercises seems like a very natural way to learn. It will be quite interesting to see how this will change during the course.

My future job prospects as a physicist will most likely revolve about programming and handling large amounts of data, regardless of whether I will pursue a career in industry or I will stay in academia. Jobs as a Data Scientist, Programmer or in the engineering direction are quite common when getting a Masters in physics and experimental physics in academia has mostly been computing, simulation or the analysis of huge amounts of data since many years already. Therefore, having a strong basis in programming, data analysis and visualization are skills one should have after the studies. I expect that this course will deepen my knowledge in Data Mining by not only introducing new concepts but also connecting those learned already on an even deeper level and will thus be a helpful resource for my future.

I will use Large Language Models in the following mainly for getting code suggestions for the exercises and help in the layout of this report (as LaTex can be rather cumbersome at times). The text will mainly be written by myself, although sometimes AI is used for translation and paraphrasing purposes. All code of the exercises as well as the LaTex files to create this report will be made available on a public GitHub repository [1].

2. Introduction and basics

Lecture

The lectures this week dealt with introductory topics regarding the structure of this course, a math and statistics rehearsal as well as an introduction to the topic Data Mining. The math and statistics chapter covers many basic definitions like the axioms and basics properties of probabilities, the definitions of partial derivatives, vectors and matrices and their addition and multiplication properties. Although these are nice to have for completeness sake and should prove helpful for students which do not have a background in statistics yet, for me, they were already known and will therefore not be repeated here. Instead, I will focus on definitions of this chapter which I do not know by heart and which I think will prove useful for the following and will put them into context of what I have already learned.

The sample mean $\hat{\mu}$ and sample variance $\hat{\sigma}^2$ provide unbiased estimators for the population mean μ and population variance σ^2 given a certain sample v_i of size N, i.e. $i \in (1, N)$. They are defined as

$$\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} v_I \tag{1}$$

$$\hat{\sigma}^2 = \frac{1}{N-1} \sum_{i=1}^{N} (v_i - \hat{\mu})^2 \tag{2}$$

I recall from a prior course on statistics that the sample variance with the $N - 1$ term in the denominator should be used in the case of an *unknown* mean, i.e. if the mean is estimated by Equation 1, as it provides an unbiased estimator and therefore better convergence to the true but unknown sample variance for small N. If instead the mean is inferred through different means, the minus 1 term can be dropped. In `numpy` the sample variance can be simply calculated by setting the parameter `ddof=1`:

```
    import numpy as np
    # array is a sample array of data
    sample_var = np.std(array, ddof=1)
```

Listing 1: Sample variance, calculated in numpy

If there are more than just one random variates a variance can be calculated for each one. Additionally, a so-called covariance between two different variated can also be calculated. Covariances and variances are summarized in a covariance matrix, whose elements are defined as follows:

$$\mathrm{Cov}\left(x, y\right) = \frac{1}{n-1} \sum_{i=1}^{N} \left(x_i - \hat{\mu}_x\right)\left(y_i - \hat{\mu}_y\right) = \hat{\sigma}_x \hat{\sigma}_y \rho_{x,y} \tag{3}$$

Here $\hat{\sigma}_i$ are the standard deviations of the variates x and y according to Equation 2 and $\rho_{x,y}$ is the degree of correlation between x and y. It holds that $\rho_{x,y}$ is always between -1 and 1 with -1 indicating maximum negative correlation, 1 maximum positive correlation and 0 no correlation at all. The covariance matrix (or the reduced correlation matrix obtained when removing all individual standard deviations) therefore indicates correlations between different parameters in a dataset which can be used for explorative data analysis. Another use of it is when fitting a model to a dataset. Here a large degree of correlation between model parameters indicates a surplus of model parameters.

The normal distribution is the most important continuos probability distribution as a lot of measured data follows it. This is due to the central limit theorem stating that means of random variables taken from arbitrary probability distributions will be distributed normally. As measured quantities are usually means over some finite measurement integration time due to a finite detector resolution many data are distributed normally. The normal or Gaussian probability distribution is given by

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{4}$$

with μ its mean and σ its width, corresponding to the population standard deviation in x. It is a symmetric distribution and used to formulate confidence intervals as follows:

$$\begin{aligned} P\left(\mu - 1\sigma < x < \mu + 1\sigma\right) &\approx 68\% \\ P\left(\mu - 2\sigma < x < \mu + 2\sigma\right) &\approx 95.5\% \\ P\left(\mu - 3\sigma < x < \mu + 3\sigma\right) &\approx 99.7\% \end{aligned} \tag{5}$$

Further important definitions are those of the Jacobian and Hessian matrices, which are matrices of first order derivates of vector valued functions $\mathbf{f}(\mathbf{x})$ or second order derivates of scalar valued functions $f(\mathbf{x})$ respectively. They are used in optimization algorithms like data fitting or neural network learning. These methods are usually implemented already in various Python packages, however I still list the form of the Jacobian and Hessian here for completeness:

$$\mathbf{J} = \nabla_x \cdot \mathbf{f}(\mathbf{x}) \qquad \text{or element-wise:} \qquad J_{ij} = \frac{\partial f_i}{\partial x_j} \tag{6}$$

$$\mathbf{H} = \nabla_x^2 f(\mathbf{x}) \qquad \text{or element-wise:} \qquad H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j} \tag{7}$$

The last part of the lecture considered Data Mining. We discussed that Data Mining is a very structured process, where certain steps are done in order to hopefully get meaningful insights from the data at hand and be able to form a model that generalizes well. The first step is explorative data analysis (EDA), where plotting the data (e.g. in histograms or box plots) or calculating covariance matrices to get a rough idea about correlation are utilized. This step makes a lot of sense to me, especially once one deals with larger and larger datasets. However, this has been quite underutilized during my physics studies so far, as we have usually worked the other way around by first forming a hypothesis (for example a model) and then applying it to the data and doing statistics to see if it fits. It is quite interesting to me to do a different approach in this lecture and to see, where this may lead me. I am looking forward to applying this to real datasets in the following weeks during the tutorials. The next step is descriptive modelling, where one tries to find patters in the data by, fundamentally, playing around with it. One can for example try to fit functions like multivariate Gaussians or use

at end: see if this really was interesting!

clustering methods on the data. Additionally, one can also try to use predictive modelling like classification neural networks to group the data and gather new insights. Hopefully these steps then lead to discovering patterns and rules in the data and finding a strong, i.e. simple model with high degree of generalization and prediction-power instead of remaining with weak models, which do offer some insights but fail to generalize and really understand the data. Weak models are also often classified by many parameters leading to the aforementioned overfitting. During my prior classes where I often used model fitting and machine learning I have often had contacts with overfitting due to fit functions with too many free parameters or overly large neural networks. I therefore know, that avoiding overfitting is one of the most difficult parts in data analysis and am definitely looking forward to learning more about this.

Exercise

Reflection

1. how was learning this week?
2. How was writing the diary?

3. Environmental data and its pre-processing

4. Data visualization

5. Clustering in Python

6. Predictive modeling

7. Summary

8. Self-evaluation

References

[1] Stephen Weybrecht. *Data Mining in Environmental Science: Repository.* `https://github.com/stewey0/uef-data-mining`. Source code. Accessed: November 18, 2025.