Chapter 3: An introduction to Machine Learning (STK353)

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Section 1

Initial concepts

Structured data vs unstructured data

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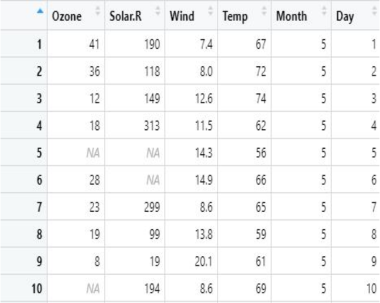
- **Web data**: Web pages, HTML documents, web logs and etc.

What is a data set?

A data set is a collection of data objects and their attributes.

- Attribute is also known as variable, field, characteristic, or feature.
- Object is also known as record, point, case, sample, entity, or instance.



	Ozone	Solar.R	Wind	Temp	Month	Day
1	41	190	7.4	67	5	1
2	36	118	8.0	72	5	2
3	12	149	12.6	74	5	3
4	18	313	11.5	62	5	4
5	NA	NA	14.3	56	5	5
6	28	NA	14.9	66	5	6
7	23	299	8.6	65	5	7
8	19	99	13.8	59	5	8
9	8	19	20.1	61	5	9
10	NA	194	8.6	69	5	10

Figure 1: A dataset.

Explanatory variables vs. Response variable

Explanatory variables (also known as input variables, features, or independent variables) and response variables (also known as output variables or dependent variables) play distinct roles in the modeling process. Here's an explanation of each:

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The goal of the machine learning model is to learn a mapping or relationship between the explanatory variables and the response variable, enabling it to make predictions or classifications on new data.

Section 2

Machine learning: What, why & when

What is Machine Learning?

The foundation of machine learning lies in the idea that computers can learn patterns and make predictions based on data.

Coined by Samuel in 1959, the term machine learning (ML) was given to the field of study of the development of algorithms and models that can automatically learn patterns and make predictions or decisions based on data. It is a subset of artificial intelligence (AI) that aims to enable machines to improve their performance over time by using experience.

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- Algorithms: Machine learning algorithms are used to analyze and process the data, extract patterns, and make predictions or decisions. These algorithms can be categorized into supervised learning, unsupervised learning, semi-supervised learning, and reinforcement learning.

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- Models: Machine learning models are the result of training algorithms on data. These models can be used to make predictions or classify new data.

Why do we use Machine learning?

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- **Medical Diagnosis and Healthcare:** Machine learning models can assist in medical diagnosis by analyzing patient data and identifying patterns that may indicate diseases or conditions. They can aid in early detection and personalized treatment plans.

Machine learning vs. Statistical learning

While machine learning and statistical learning share common techniques and goals, they differ in their focus, approach, and emphasis. Machine learning emphasizes practical applications, scalability, and prediction accuracy, while statistical learning focuses on understanding relationships, making inferences, and assessing uncertainty. Both fields have their strengths and are often used in complementary ways to solve a wide range of problems.

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    - Statistical Learning: Statistical models, on the other hand, are designed for inference about the relationships between variables. Many statistical models can make predictions, but predictive accuracy is not their strength. Statistical learning focuses on understanding and modeling complex relationships in data using statistical techniques. It aims to make inferences and draw conclusions about the underlying processes that generate the data.

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- Machine Learning: Machine learning often employs a more algorithmic and computational approach, utilizing techniques such as neural networks, decision trees, support vector machines, and deep learning. It emphasizes optimization, generalization, and scalability. Machine learning algorithms are designed to automatically learn patterns and relationships from data, often with less emphasis on the underlying statistical assumptions.

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   - Statistical Learning: Statistical learning focuses on understanding the underlying statistical properties of the data and making inferences based on those properties. It utilizes techniques such as linear regression, logistic regression, Bayesian methods, and hypothesis testing. Statistical learning often involves making assumptions about the data distribution and relies on statistical theory to draw conclusions and make predictions.

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- Machine Learning: Machine learning algorithms can handle a wide range of data types, including structured, unstructured, and high-dimensional data. They often require large amounts of labeled data for training and can handle noisy or incomplete data. Machine learning algorithms are generally more flexible and can adapt to different data distributions without strict assumptions.

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- Statistical Learning: Statistical learning techniques often assume that the data follows a specific probability distribution or statistical model. They are more suited for structured data and often require assumptions about the data's distribution, independence, and linearity. Statistical learning methods may struggle with high-dimensional or unstructured data and may require more careful preprocessing and feature engineering.

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- Statistical Learning: Statistical learning places a stronger emphasis on understanding the underlying relationships and making inferences about the data. It aims to draw conclusions about the significance and effect of variables, estimate parameters, and assess uncertainty. Statistical learning methods often focus on hypothesis testing, confidence intervals, and interpreting the coefficients of the model.

5. **Higher accuracy in prediction vs. interpretability**

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- Statistical learning models, such as linear regression or logistic regression, often have a clear and interpretable structure. They provide coefficients or parameter estimates that can be directly interpreted to understand the relationship between input variables and the target variable.
- These models are often based on well-established statistical principles and assumptions, allowing researchers to make inferences about the significance and effect of variables.
- Statistical models are commonly used in scientific research, where interpretability is crucial for understanding the underlying processes and drawing meaningful conclusions.
- Machine learning models, such as deep neural networks or ensemble methods, are often more complex and have a larger number of parameters. This complexity can make them less interpretable compared to statistical models.
- The focus on accuracy may lead to models that are more black-box in nature, making it challenging to understand how the model arrives at its predictions.

Trade-off between Interpretability and Accuracy:

- There is often a trade-off between interpretability and accuracy in machine learning. As models become more complex and flexible, they can achieve higher accuracy but at the cost of reduced interpretability.
- In some cases, interpretability may be less important, such as when the primary goal is to achieve the highest possible accuracy in tasks like image recognition or natural language processing.
- However, in domains where interpretability is crucial, such as healthcare or finance, simpler and more interpretable models like decision trees or logistic regression may be preferred, even if they sacrifice some accuracy.

Various types of machine learning algorithms

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1. **Supervised Learning:** Here we have a clearly defined response variable (or variables) Y and a set of explanatory variables $\mathbf{X} = (X_1, \dots, X_d)$ and the goal is to find the relationship between Y and $\mathbf{X}$ in order to perform statistical inference, prediction, etc. The response variable is like a teacher in this type of problems and it is used to supervise us and show us our mistakes until we get good at what we do. In supervised learning, when the response Y is a quantitative variable (i.e. it takes numerical values), we are dealing with a regression problem. And when the response Y is a qualitative or categorical variable (i.e. it takes finitely many discrete values, in other words, its values belongs to one of finitely many classes or categories), we are dealing with a classification problem.

2. **Unsupervised Learning:** Unsupervised learning involves training models on unlabeled data, where the algorithm learns to find patterns and structures in the data without any predefined labels. Indeed, here, there is no clearly defined objective and we often do not have a predefined response variable Y (we have only observed the input variables). So, nothing is there to supervise us and the ultimate goal is to explore the data and look for interesting patterns in the data. In these settings we may for example be interested in detecting patterns in the data. Usually, this is the starting point to perform a subsequent supervised learning. Clustering and dimensionality reduction (e.g. PCA) are common tasks in unsupervised learning.

3. **Reinforcement Learning:** Here the ultimate goal is to develop learning system that receives a reward signal and tries to learn to maximize the reward signal. It has been applied to problems such as game playing (playing chess with the computer), robotics, and autonomous driving. We do not consider this type of learning in this course but feel free to consult with the book Reinforcement Learning: An Introduction by Sutton and Barto (2018).

Section 3

Additional concepts in machine learning

Experimental design in machine learning

It refers to the process of setting up and conducting experiments to evaluate the performance of machine learning models. It involves various steps, including splitting the dataset into training and test sets, selecting appropriate performance metrics, and utilizing techniques like cross-validation. Let's explore each of these components:

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1. **Splitting the dataset:** To evaluate the performance of a machine learning model, it is crucial to divide the available dataset into two separate sets: the training set and the test set. The training set is used to train the model, while the test set is used to assess its performance on unseen data. The typical split is around 70-80% for training and 20-30% for testing, but this can vary depending on the size of the dataset.

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2. **Performance metrics:** Performance metrics are used to measure how well a machine learning model performs on the test set. The choice of metrics depends on the specific task and the nature of the data. For classification tasks, common metrics include accuracy, precision, recall, F1 score, and area under the ROC curve. For regression tasks, metrics like mean squared error (MSE), mean absolute error (MAE), and R-squared are commonly used.

Cross-validation:

Cross-validation is a technique used to assess the performance of a model and mitigate the potential bias introduced by a single train-test split. It involves dividing the dataset into multiple subsets or “folds.” The model is trained and evaluated multiple times, with each fold serving as the test set while the remaining folds are used for training. This helps to obtain a more robust estimate of the model’s performance.

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- **k-fold cross-validation:** In k-fold cross-validation, the dataset is divided into k equal-sized folds. The model is trained and evaluated k times, with each fold serving as the test set once. The performance metrics are then averaged across the k iterations to obtain a more reliable estimate of the model’s performance.

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- **Leave-one-out cross-validation:** Leave-one-out cross-validation is a special case of k-fold cross-validation where k is equal to the number of samples in the dataset. Each sample is used as the test set once, while the remaining samples are used for training. It can be computationally expensive but provides an unbiased estimate of the model's performance.

Over fit vs. Under fit vs Good fit

- Overfitting: Overfitting is like a student who memorizes the exact answers to specific practice questions but fails to understand the underlying concepts. When faced with new test questions that require applying those concepts in a different way, the student struggles. Similarly, in machine learning, an overfit model memorizes the training data too closely but fails to generalize well to new data.

- Underfitting: Underfitting is like a student who doesn't study enough and lacks a solid understanding of the subject. They may perform poorly on both practice questions and new test questions because they haven't grasped the fundamental concepts. In machine learning, an underfit model is too simplistic and fails to capture the underlying patterns in the data, resulting in poor performance on both the training data and new data.

- Good fit: A good fit is like a student who strikes the right balance between memorization and understanding. They study the materials, grasp the core concepts, and can apply them to a variety of questions. This student performs well on both practice questions and new test questions because they have a solid foundation. Similarly, in machine learning, a good fit model captures the underlying patterns in the data without being too specific or too simplistic, allowing it to generalize well to new data.

Section 4

Supervised learning

Section 5

Unsupervised learning