



Notes on
Machine Learning Lecture

Taught by
Prof. Dr. Joni Dambre
Prof. Dr. Tom Dhaene

Created by
M.Sc. Student
Karina Chiñas Fuentes

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DISCLAIMER

These are my notes and associated further reading that regards my understanding of Machine Learning based on the Universiteit Gent 2022 winter lecture. Non-cited statements come from the lecture. I also make notes to myself. If the reader finds something useful, I encourage them to investigate further. Non-cited charts were created by me, and their nonprofit-related usage is allowed with a citation.

The following text is from me to me; to prepare myself for the examination and enhance my knowledge of related topics.

Before you redact:

1. What are the keywords?
2. What are the assumptions of the model or algorithm?
3. What are the main take away?
4. Flow Charts?
5. Advantages and Disadvantages
6. Are they linear or non-linear transformations / models

1 First Steps in Supervised Learning

1.1 What is Machine Learning?

Machine Learning is the field that generates algorithms that learn from data so they can predict or make decisions based on their learning. One aims to **build a model for data by optimizing the performance criterion using training data**. See Figure 1 for the different fields surrounding machine learning.

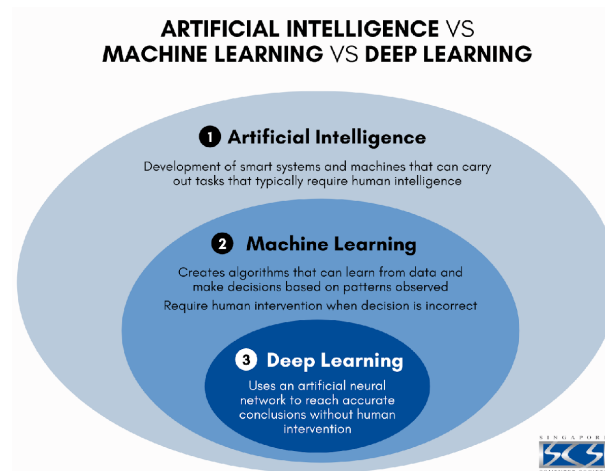


Figure 1: Surrounding fields in Machine Learning. Image from [1].

To understand machine learning algorithms, it is necessary to know about Probability Theory and Statistics. It is also desired to have efficient programming knowledge, so this is an interdisciplinary field.

Learning algorithms are implemented when no rules are available to establish the relationship between the input and the output. It is also possible that the algorithm is required to adapt to different environments.

1.2 Types of Machine Learning

There are three main different types of machine learning; these are depicted in Figure 2.

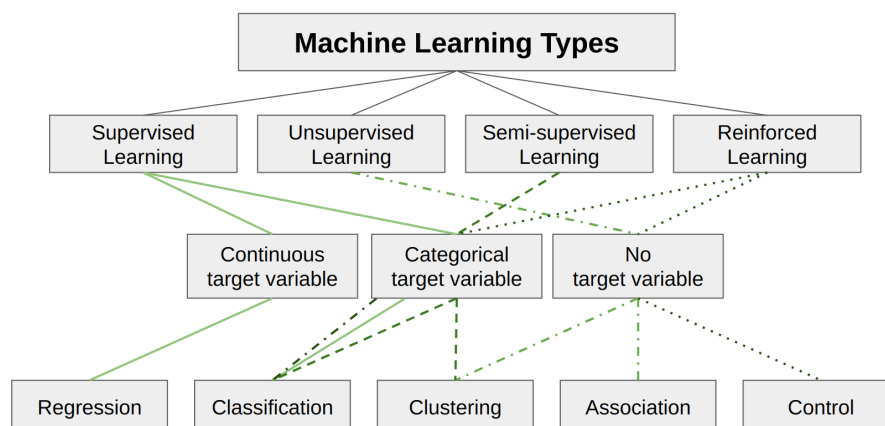


Figure 2: Different types of machine learning. Image inspired from [2].

- **Supervised:** here, the expert gives the algorithm the output data (as labels for classification) so that the input-output relationship can be modeled. The type of tasks covered here are:
 - Regression: when the output is numerical.

- Classification: when the output is categorical.
- **Unsupervised:** the aim is to learn without an output; this approach allows us to model the structure of the data or the underlying profile of the data; they can become *discriminative* or *generative*¹; for instance, Gaussian mixture models², random forests, and neural networks are discriminative models. Generative models are often used as pre-processing in deep learning [4].
 - Clustering: hierarchic and nonhierarchic are their sub-branches; more might be investigated. Clustering can be both discriminative and generative.
 - Association / Transformation of Features: the aim is to uncover latent variables or compress information. This can either improve or worsen the interpretability of the model, e.g. Principal Component Analysis (PCA); see Figure 3.

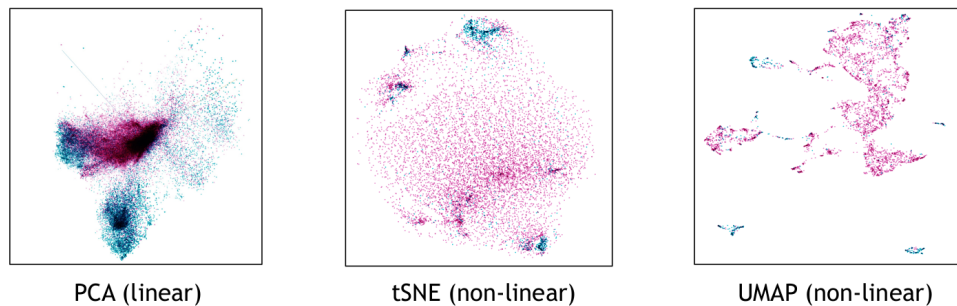


Figure 3: Different types of feature transformation, showing PCA (left), t-Distributed Stochastic Neighbor Embedding (center), and Uniform Manifold Approximation and Projection (right). Image inspired from lecture 1.

- **Semi-supervised Learning:** as the name suggests, this is a mixture of the previous two and is typically implemented when the cost of labeling is high [2].
- **Reinforced Learning:** this method uses gathered information from the interaction with the environment to maximize reward and reduce risks [2]; this can be implemented for real-time decisions.

1.3 Supervised Learning

The notation used in this document is the following:

- Ground truth: $\mathbf{y} = f(\mathbf{x}) + \varepsilon$
- Training data: $\mathbf{X}, \mathbf{Y} : (\mathbf{x}_1, y_1), \dots (\mathbf{x}_N, y_N)$
- Hypothesis: $f(\mathbf{x}) \sim g(\mathbf{x}, \mathbf{X}, \boldsymbol{\theta}) + \varepsilon$; best model that can be learned from a certain model family.
- Loss function: $\mathcal{L}(\boldsymbol{\theta} | \mathbf{X})$
- Learning: $\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} (\mathbb{E} [\mathcal{L}(\boldsymbol{\theta} | \mathbf{X})])$; minimize expected loss on new data.

Notice that $f(\mathbf{x})$ is unknown. In general, finding the optimal parameters that will minimize the expected loss function on new data is necessary. Optimal parameters depend on the assumption made on data. Finding non-parametric algorithms in supervised learning for regression and classification is also possible, e.g., K-nearest neighbors (KNN). See Figure 4 for a better comparison.

! Algs: KNN (regression and classification), decision trees (regression and classification), linear discriminate (regression and classification), and non-linear feature expansion (regression).

Consider mentioning the training/inference time and memory scale w.r.t. dataset size when describing an algorithm. These issues become relevant once the quality of the data has been addressed.

¹The algorithm focuses on devising the decision boundary (without underlying assumptions on data) or on modeling the joint distribution of inputs and outputs, respectively.

²See more in [3].

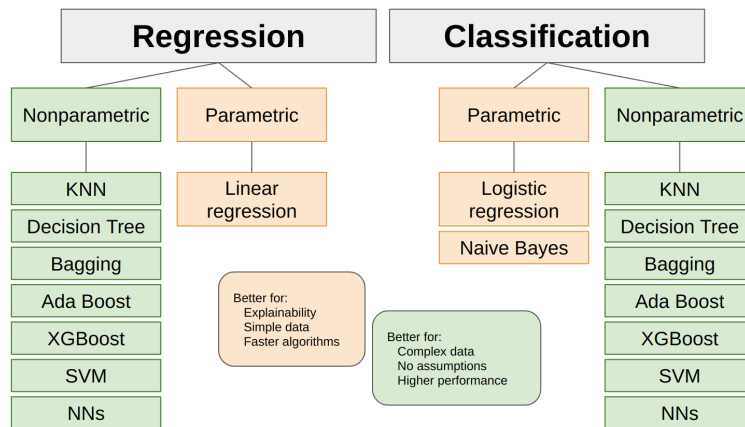


Figure 4: Types of algorithms in supervised learning and some examples. Image inspired from [5].

1.4 Evaluating Models and Conditions for Generalization

Machine learning aims to achieve **generalization**; the algorithm should perform well when new data is introduced. To understand how this is feasible, important concepts will be introduced.

- **Loss function:** this is among the most important metric in machine learning. This function allows the user to tell how good a model's prediction is, based on the *the loss*. This transforms the learning into an optimization problem by defining a loss function and optimizing it to its minimum. More on this shall be explored [6]. **!** Different loss functions, different predictions.
- **Empirical Risk Minimization (ERM):** the understanding of ERM permits us to understand the limits of an algorithm, which also allows the development of practical skills in machine learning [7]. The concept of empirical risk arises from the fact that the user cannot access the *true error* since the algorithm only receives a sample of an unknown distribution from the data. However, estimating the *training error* – the error the algorithm incurs over the training sample [8] is possible. In short, ERM is the search for a predictor (or model) that minimizes the training error; this can be depicted in the following expression

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} \left(\frac{1}{N} \sum_{j=1}^N \mathcal{L}(x_j | \theta, \mathbf{X}) \right). \quad (1)$$

Remember that the model represents your **hypothesis**. ERM: the search for the best model that minimizes training error.

- **Test Error:** because the ERM does not tell the user how well the algorithm is capable to predict on new data, what is typically done is to split the available data such that, once the algorithm has been trained (found $\hat{\theta}$), the algorithm can be assessed on the performance on the *test data*. **!** WARNING: depending on how you split the data, how likely you are introducing *leakage* in your model.
- **redo IID Assumption:** Identically and Independent Assumption:
 - Indetically: training, validation, test, and new incoming data are drawn from the same underlying joint distribution. In other words, all datasets must have the same statistical properties: mean, standard deviation, and other characteristics [9].

Violating this assumption creates

- * prediction bias; predictions are not characteristic of the real world due to lack of representative groups, e.g., training facial recognition on engineering students: population not very diverse, very few women, no children, no elderly people. This can also result from lack of balanced classes.

Feature and label bias can be considered a violation of the “identically distributed” part of the i.i.d. assumption.

- Independent: no subgroups of samples correlated in any type of data subset (training, validation, and test); in other words, any data point should not provide information on the occurrence or value of another data point [9]. Usually, The correlation is attributed to **latent variables**, a.k.a. unknown or unobserved variables.

Violating this assumption creates

- * bias;

Violation of any assumption leads to poorer generalization, and they can be interconnected. **!!!** I think what is important in this discussion is identifying the source of a violation rather than the independent consequence because the violation of each might result in a similar consequence. **FOCUS ON THE SOURCE RATHER THAN THE CONSEQUENCE.**

For instance, the characteristic clusters in **STDB5** for the spherical and non-spherical tokamaks violate the identical assumption. This might not necessarily mean that spherical tokamaks must have their own scaling law (?). In reality, there is no continuum in aspect ratio to effectively assess whether they are *identical* machines. This implies too much money to discover.

1.5 Model Selection: hyperparameter analysis

When one changes the hyperparameters of an algorithm, it can be considered a different model than before; for instance, the number of features one uses is a hyperparameter. How can one tell which model is better compared to another? It is recommended to follow the diagram shown in Figure 5, left.

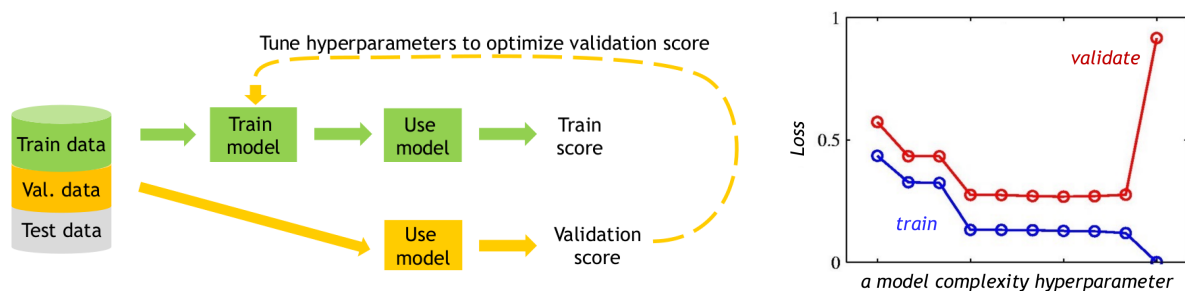


Figure 5: Left: data split for model assessment, all data subsets are assumed to follow IID assumption. Right: validation curve; if the IID assumption is not fulfilled, the curves will not look similar; this is why it is recommended to look at this plot at the beginning. Sometimes, the validation curve is plotted with accuracy or another metric, like F_1 -score. Images from lecture 1.

When you tune the model's hyperparameters, you also change the model complexity; the validation curve is assessed from this analysis. The validation curve plots a model performance metric vs. the algorithm's complexity [10]. The typical behavior is that the validation error goes down as the complexity increases, but the error goes up again at some point; see Figure 5, right. **More on this will be explained when the bias-variance decomposition in a model is studied.** Once the ideal model has been found, the train and validation datasets are merged to obtain the overall train and test errors without further modification. This is depicted in Figure 6

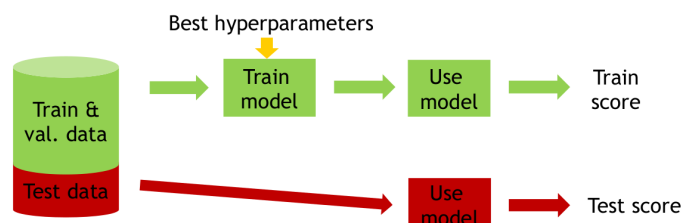


Figure 6: Data split for model assessment, final stage. Image from lecture 1.

If the validation and training data are too small, the model will likely have a poor choice of hyperparameters and might overfit. Again, beware of how you split the data, as you might introduce a source of leakage.

Another discussion brought on the analysis of model complexity is the choosing of features. In general, it is not ideal to have too many features due to what is known as *the curse of dimensionality*. The reasoning is that a higher number of features implies a more complex model, and the more complex the model, the more data it requires to perform well. For instance, consider the case of fitting data with a polynomial of degree d with F total number of features. The complexity of the said model is $\mathcal{O}(F^d)$; from this, it is possible to observe that the selection of features becomes a serious matter for optimal performance, directly affecting its generalization capability.

Here are some forms of **regularization** for optimal model selection:

- Spend time searching for the optimal subset of features to avoid the "curse of dimensionality".
- If possible, reduce the number of hyperparameters (this is a matter in neural networks).
- Constrain parameter space: the idea is that you assess for a region in parameter space where you know solutions will lead to an optimal generalization, e.g. L_1 and L_2 regularization, more on this in the incoming chapter.
- When working with optimization algorithms, such as gradient descent, avoid over-tuning in training data (e.g. early stopping).

1.6 Summary

Key words: empirical risk minimization (ERM), validation curves, curse of dimensionality.

2 Supervised Parametric Linear Models and Introduction to SVM

2.1 Linear Models Nomenclature

A linear discriminant is essentially ordinary least squares, which can be expressed as

$$g(\mathbf{x} \mid \boldsymbol{\theta}) = g(\mathbf{x} \mid \mathbf{w}, w_0) = \mathbf{w}^T \mathbf{x} + w_0 = \sum_{j=1}^d w_j x_j + w_0. \quad (2)$$

Here, the model parameters enclosed by $\boldsymbol{\theta}$ are the weights \mathbf{w} plus a *bias*³, w_0 . Just like the scaling law of the energy confinement time, w_0 accounts for α_0 ; however, here, one can make a distinction between the dataset accounting for the intercept or not, as follows:

³The term "bias" is heavily used in machine learning, so be sure that you know well the context when discussing bias.

$$\tilde{\mathbf{X}} = (\mathbf{1}, \mathbf{x}_1, \dots, \mathbf{x}_F); \text{ and } \mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_F) \quad (3)$$

as well as $\boldsymbol{\theta} = \tilde{\mathbf{w}} = (\mathbf{w}_0, \mathbf{w}_{11}, \dots, \mathbf{w}_{F_F})$, so the compact notation of Eq. (2) becomes $g(\mathbf{x} | \boldsymbol{\theta}) = \tilde{\mathbf{w}}^T \tilde{\mathbf{X}}$. **!** WARNING: not to be confused with OLS for scaling law of confinement time's notation.

Positive aspects of OLS: easy implementation, easy interpretation, and cheap computational power. Inference's complexity is $\mathcal{O}(F)$ linearly dependent on the number of features.

Remember that explicitly evaluating the expected loss is inaccessible; hence, the ERM is implemented, which implies the need for a loss function.

2.2 Loss Functions for Regression: where do they come from?

The probabilistic, or statistical, view of regression introduces the sum squared errors (MSE). The assumption on linear regression (OLS) is that the ground truth contains irreducible error given by $\varepsilon \sim \mathcal{N}(0, \sigma^2)$; where the standard deviation σ is constant. If the data matches this assumption, statistical tests hold their intended interpretation (e.g. the existence of uncertainty margins). From this, it follows that

$$\varepsilon = \mathbf{y} - f(\mathbf{x}) \sim \mathcal{N}(0, \sigma^2), \quad (4)$$

but, $f(\mathbf{x})$ is approximated through the model $g(\mathbf{x} | \boldsymbol{\theta})$. In other words, the assumption implies that the probability of finding the correct prediction is normally distributed with

$$p(y | \mathbf{x}) \sim \mathcal{N}(g(\mathbf{x} | \boldsymbol{\theta}), \sigma^2); \quad (5)$$

this is shown in Figure 7.

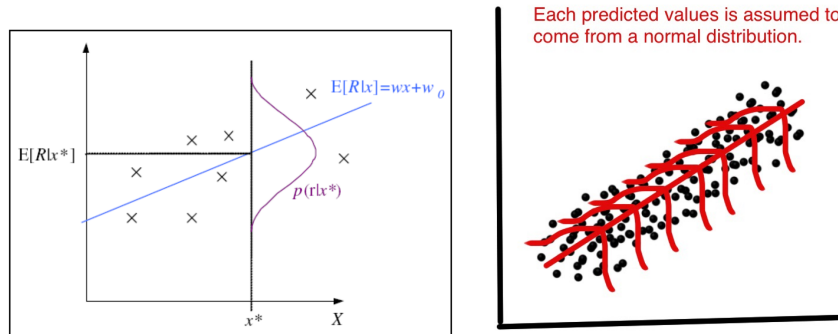


Figure 7: Linear regression, statistical interpretation. Here $r = y$. Right image is from [11], left image is from lecture 2.

This is optimized through the maximum likelihood (ML) approach for one specific output. So, the likelihood of one training example with normally distributed error implies

$$p(y_t, \mathbf{x}_t | \boldsymbol{\theta}) \sim \mathcal{N}(g(\mathbf{x}_t | \boldsymbol{\theta}), \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2\sigma^2} (g(\mathbf{x}_t | \boldsymbol{\theta}) - y_t)^2 \right]. \quad (6)$$

Hence, the joint likelihood for all training examples in the dataset takes the following form

$$p(\mathbf{y} | \mathbf{X}, \boldsymbol{\theta}) = \prod_{t=1}^N p(y_t, \mathbf{x}_t | \boldsymbol{\theta}) \sim \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right)^N \prod_{t=1}^N \exp \left[-\frac{1}{2\sigma^2} (g(\mathbf{x}_t | \boldsymbol{\theta}) - y_t)^2 \right]. \quad (7)$$

!! NOTICE that the first equality assumes independence among observations in accordance with the IID assumption.

Now, remember from basic calculus that when finding a function's minimum or maximum, one needs to take the second derivative of such function and equate it to zero. This approach is also used to find the maximum joint likelihood. However, because here one deals with more than one parameter (or feature), one needs the expression of *gradient*; namely, the column vector defined as

$$\nabla_{\theta} = [\partial_{w_0}, \partial_{w_1}, \dots, \partial_{w_F}]^T. \quad (8)$$

To ease the mathematics, one can take the negative logarithm of Eq. (7), such that

2.3 Loss Functions for Classification

2.4 Learning parameters for MSE and Logloss

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2.5 DEMON: Gradient descent for linear regression

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2.6 Overfitting and Regularization

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2.7 Maximal Margin Classification – Linear SVM

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2.8 Maximal Margin Classification – Soft Margin (linear)

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2.9 Summary

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3 Reasoning About Models and Data

3.1 Error Functions for Model Selection

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3.2 Bias and Variance

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3.3 Data Splitting and IID

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3.4 Robust Validation Strategies

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3.5 Analysis of Model Performance

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3.6 Augmentation

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3.7 Summary

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4 Clustering – K-Means and Clustering Mixture Models

4.1 Latent Variables

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4.2 K-Means Clustering

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4.3 Mixture Distributions: Mixture of Gaussians

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4.4 Expectation-Maximization (EM) Algorithm

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4.5 Summary

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5 The Data Pipeline (DP) and Ramp-Up Towards Non-Linear Models

5.1 DP Cleaning

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5.2 DP Feature Extraction / Expansion

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5.3 DP Transformations and Embeddings

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5.4 DP Dimensionality Reduction

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5.5 Introduction to Kernels

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5.6 Summary

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6 Directed and Undirected Graphical Models

6.1 Directed Graphical Models: Bayesian Networks

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6.2 Undirected Graphical Models: Markov Random Fields

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6.3 Inference in Graphical Models

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6.4 Summary

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7 Bayesian Estimation

7.1 Regression

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7.1.1 Polynomial Fitting

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7.1.2 General Least-Squares

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7.1.3 Overfitting Problem

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7.1.4 Ridge Regression

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7.2 Probability Concepts

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7.3 A Probabilistic View on Regression

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7.3.1 Least-Squares Estimation as Maximum Likelihood

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7.3.2 Maximum-A-Priori (MAP) Estimation

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7.3.3 Bayesian Curve Fitting

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7.4 Summary

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8 Hidden Markov Models and Gaussian Processes

8.1 Introduction

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8.2 Models for Sequential Data

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8.3 Hidden Markov Models

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8.4 Extensions

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8.5 Introduction to Gaussian Processes

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8.6 Regression

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8.6.1 Covariance Function

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8.6.2 Prediction

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8.6.3 Implementation

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8.6.4 Hyperparameters

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8.6.5 Sequential Sampling

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8.7 Optimization

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8.8 Classification

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8.9 Summary

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9 Combining Multiple Learners – Ensembles

9.1 Introduction

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9.2 Bagging, Boosting, and AdaBoost

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9.3 Loss Function and Viola-Jones Face Detector

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9.4 Decision Trees: CART Framework

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9.5 Random Forests

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9.6 Summary

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10 Neural Networks and Feature Learning

10.1 Introduction

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10.2 Multi-Layer Perceptrons (MLP)

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10.2.1 Back Propagation

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10.3 Convolutional Neural Networks (CNN)

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10.4 Overfitting and Regularisation

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10.5 Auto-encoders and Embeddings

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10.6 Deep Learning Extensions

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10.7 Recurrent Neural Networks

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10.8 Summary

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11 Ethical Aspects in Machine Learning

11.1 Examples of Powerful Algorithms and Ethical Concerns

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11.2 Overconfidence and Unreliability of Models

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11.3 Model Explainability

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11.4 FAIRNESS: Criteria, Mitigation & “Fairness by Awareness”

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11.5 Summary

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