40 Algorithms Every Data Scientist Should Know

Navigating through essential AI and ML algorithms

Jürgen Weichenberger

Huw Kwon

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Dedicated to

My beloved wife: ***Li*** *and*

My Daughter ***Sophia***

– Jürgen

Ross McDonald, Matthew Jones, Edward Huang, Neil Graham, Raj Dash, Mark Somers, Philip Treleaven, Mark Rowland, Matt O'Kane, Andy Huang, Huw Tindall, Luigi Masoero, Michael Glinski, Gerard Crispie, Rob Handcock, George Marcotte

and the three professors named ***Alan*** *at the University*

– Huw

About the Authors

- **Jürgen Weichenberger** has been working in Artificial Intelligence and Machine Learning Development for more than 20 years, playing central roles in numerous projects as a technical leader and chief data scientist, delivering projects using numerous different algorithms and even developing entire new algorithms for big companies, including well succeeded projects in Europe, Asia, and North America. Currently, he is a Head of AI Strategy and Innovation at Schneider Electric and a Senior Advisor at P.E.T. Consulting. He is also an accomplished postgraduate completing a degree in Executive General Management and holds three master's degrees focused on Applied Computer Science, Bioinformatics, and Cybernetics. He has many certifications for various types of Artificial Intelligence Technologies. Furthermore, the author participates as a speaker in international AI Conferences and writes technical articles on AI Technologies, Algorithms and related topics. Based on all his contributions to AI communities worldwide, he was awarded over 20 AI patents.

- **Huw Kwon** is a well-known authority in AI and ML within the management consulting world, bringing over two decades of academic rigor and truly extensive practical experience to the field as a first-hand practitioner. With a strong foundation in management science and advanced computational algorithms, his work is unified by a singular focus: leveraging AI to create tangible, sustained, and lasting real-world impact.

  Huw's career spans senior roles in banking and consulting at some of the world's most prestigious firms, including Ernst & Young, Accenture, and McKinsey. In these roles, he has been pivotal in transforming businesses by developing AI capabilities and leading complex, large-scale transformation programs across industries such as financial services, automotive, and high-performance manufacturing.

  As a member of several advisory boards and a recognized thought leader, Huw frequently contributes to industry forums and publications, shaping the discourse on the future of AI. Beyond consulting, he is a driving force in AI innovation, working closely with academic institutions and startups to push the boundaries of what AI and ML can achieve in practical applications.

About the Reviewer

Dr. Zachary Elewitz is a data scientist with over a decade of experience, currently serving as the Head of AI at Fortune Brands Innovations. He holds two AI-related patents, sits on Texas A&M Commerce's Venture College Board, and serves in several AI-related groups, including the National Institute of Standards and Technology Generative AI Public Working Group. In his spare time, he is pursuing a Masters in Viking studies and enjoys snowboarding, indoor bouldering, and playing the guitar.

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Preface

Building Artificial Intelligence and Machine Learning Solutions is a complex task that requires a comprehensive understanding of the latest technologies and alogorithms available to us. Artificial Intelligence has become an increasingly powerful tool over the last couple of years and as such the amount of algorithsm available to us have explode.

This book is designed to provide a comprehensive guide through the world of Artificial Intelligence Algorithms and be a practical and hands-on support to every new data scientist as well as experienced data scientists. It covers a wide range of topics, including the basic definition of Artificial Intelligence and Machine Learning, basic data concepts, and basic and advanced algorithms for supervised, unsupervised, semi-supervised, and reinforcement learning algorithms.

Throughout the book, you will learn about the key features of every algorithm, their mathematical foundation, and how to use them to build Artificial Intelligence solutions that are efficient, reliable, and easy to maintain. You will also learn about best practices and design patterns for Artificial Intelligence solutions and will be provided with numerous practical examples to help you understand the algorithms.

This book is intended for new data scientists who want to learn which algorithms are available and how to build Artificial Intelligence solutions with them. It is also helpful for experienced data scientists who want to expand their knowledge of these algorithms and improve their skills in building robust and reliable Artificial Intelligence solutions.

With this book, you will gain the knowledge and skills to become a proficient data scientist and be able to build Artificial Intelligence solutions we hope you will find this book informative and helpful.

Chapter 1: Fundamentals – Introduction into the world of AI and ML algorithms covering a little historical extract to the origins of AI and how it has developed to what we know today. Every modern AI/ML algorithm follows a basic structure which assures that the training process will converge and the inference will deliver a reasonable result. Furthermore, it will cover the process of retraining an algorithm to refit its parameters and hyperparameters.

Chapter 2: Typical Data Structures – An AI/ML algorithm can neither be trained nor run an inference without being fed with the right data structure. The process of preparing the data is known as feature engineering and requires the right school of thought.

Chapter 3: 40 AI/ML Algorithms Overview – Introduction to 40 AI/ML algorithms, including the classification and structure for the 40 algorithms, in the following chapters.

Chapter 4: Basic Supervised Learning Algorithms – Chapters 4-11 will cover the 40 algorithms which comprise the core of the book.

This chapter covers essential supervised learning algorithms in machine learning. It starts with **Linear Regression**, a widely used method for modeling the linear relationship between input features and continuous target variables. It then introduces **Logistic Regression**, commonly used for binary classification by estimating the probability of class membership. The chapter also explores **Decision Trees**, which partition data based on feature values and are applicable to both regression and classification tasks, often forming the basis of **Random Forests—**an ensemble model combining multiple decision trees for more accurate predictions. Lastly, **Naive Bayes** is discussed, a probabilistic algorithm based on Bayes' theorem, known for its efficiency in tasks like text classification and spam filtering.

Chapter 5: Advanced Supervised Learning Algorithms – This chapter explores advanced supervised learning algorithms, starting with **k-Nearest Neighbors (k-NN)**, which predicts based on the majority vote of nearest neighbors and is effective for non-linear boundaries. It covers **Support Vector Machines (SVMs)**, which find an optimal hyperplane to separate classes or predict values by maximizing class margins. The chapter also examines **Gradient Boosting Machines (GBM)**, an ensemble method that combines weak models to build a strong predictor by focusing on errors from previous models. **XGBoost**, an optimized gradient boosting method known for its performance and scalability, is also discussed. Finally, it introduces **Neural Networks**, complex models inspired by the brain that learn intricate patterns through layers of artificial neurons, driving advancements in areas like image recognition and natural language processing.

Chapter 6: Basic Unsupervised Learning Algorithms – This chapter explores basic unsupervised learning algorithms, beginning with **K-means Clustering**, which groups data into clusters based on proximity. It also covers **Hierarchical Clustering**, which builds a tree-like structure of clusters by merging or splitting based on similarity. **Principal Component Analysis (PCA)** is introduced as a technique for reducing dimensionality while preserving key features by identifying principal components. **t-Distributed Stochastic Neighbor Embedding (t-SNE)** is discussed for visualizing high-dimensional data in lower dimensions, emphasizing local structures. Finally, **Association Rule Mining** with the **A priori Algorithm** is examined for discovering relationships between items in a dataset by identifying frequent item sets and generating association rules.

Chapter 7: Advanced Unsupervised Learning Algorithms – This chapter covers advanced unsupervised learning algorithms, including **Density-Based Spatial Clustering of Applications with Noise (DBSCAN)**, which identifies clusters of varying shapes and handles noise. It discusses **Gaussian Mixture Models (GMM)**, which model data as a mixture of Gaussian distributions to uncover subpopulations. **Autoencoders** are introduced for unsupervised representation learning and dimensionality reduction. The chapter also explores **Anomaly Detection**, which identifies rare or unusual instances using various techniques. Finally, **Latent Dirichlet Allocation (LDA)** is covered for topic modeling, discovering hidden topics in documents, and assigning topic distributions.

Chapter 8: Basic Reinforcement Learning Algorithms – This chapter covers basic reinforcement learning algorithms, starting with **Q-Learning**, which estimates optimal action values for state-action pairs through iterative updates. It then introduces **Deep Q-Networks (DQN)**, which uses deep neural networks to handle high-dimensional state spaces. **Policy Gradient Methods** optimize policy parameters directly to maximize rewards with algorithms like REINFORCE and **Proximal Policy Optimization (PPO)**. The chapter also explores **Advantage Actor-Critic (A2C)**, which combines policy gradient and value-based methods for stable learning. Finally, **Trust Region Policy Optimization (TRPO)** improves policies iteratively while staying close to the original policy using trust regions.

Chapter 9: Advanced Reinforcement Learning Algorithms – This chapter covers advanced reinforcement learning algorithms, starting with **Asynchronous Advantage Actor-Critic (A3C)**, which uses parallel agents to improve sample efficiency and learning speed. **Proximal Policy Optimization (PPO)** is discussed next, using a trust region approach for stable policy updates. **Deep Deterministic Policy Gradient (DDPG)** combines deep Q-networks with actor-critic methods for continuous action spaces, while **Twin Delayed Deep Deterministic Policy Gradient (TD3)** enhances DDPG by addressing overestimation with multiple critics and delayed updates. Finally, **Soft Actor-Critic (SAC)** is introduced, optimizing both reward and exploration using the maximum entropy framework.

Chapter 10: Basic Semi-Supervised Learning Algorithms – This chapter covers basic semi-supervised learning algorithms, including **Self-training**, where a model iteratively adds high-confidence predictions from unlabeled data to its training set. **Co-training** involves multiple models training on different data views and refining each other's predictions. **Multi-view Learning** enhances learning by using various data representations to ensure prediction agreement. **Expectation-Maximization (EM)** estimates parameters and missing labels in probabilistic models. Finally, **Graph-based Methods** propagate labels from labeled to unlabeled data using the data's structure, with techniques like Label Propagation and Manifold Regularization.

Chapter 11: Advanced Semi-Supervised Learning Algorithms – This chapter covers advanced semi-supervised learning algorithms, including **Transductive Support Vector Machines (TSVM)**, which uses both labeled and unlabeled data to learn decision boundaries. **Co-regularization** combines different regularization strategies to maintain consistency and reduce sensitivity to noisy labels. **Deep Generative Models**, such as VAEs and GANs, learn from both labeled and unlabeled data to generate new samples and representations. **Virtual Adversarial Training (VAT)** adds robustness to models by addressing adversarial perturbations from both data types. **Tri-training** trains three models on different labeled feature subsets, using their consistent predictions on unlabeled data to expand the labeled set.

Chapter 12: Natural Language Processing – Natural Language Processing (NLP) is a subfield of computer science, artificial intelligence, and computational linguistics that focuses on the interaction between computers and humans in natural language. NLP enables computers to process, understand, and generate natural language, which is the language used by humans to communicate with each other.

NLP involves developing algorithms and computational models that can analyze, interpret, and generate human language, including tasks such as language translation, sentiment analysis, text summarization, speech recognition, and language generation.

The goal of NLP is to enable computers to understand and respond to natural language in the same way that humans do, allowing for more natural and intuitive communication between humans and machines. NLP has applications in a wide range of fields, including machine translation, information retrieval, customer service, healthcare, and education.

Chapter 13: Computer Vision – Computer vision is a field of artificial intelligence and computer science that focuses on enabling computers to interpret and understand the visual world around them, similar to how humans perceive and process visual information.

Computer vision involves developing algorithms and computational models that can analyze and interpret images and videos. This includes tasks such as object detection, image classification, facial recognition, scene understanding, and image segmentation.

The field of computer vision has made significant progress in recent years, with the development of deep learning algorithms and convolutional neural networks, which have led to breakthroughs in tasks such as image recognition and object detection.

Computer vision has many applications in various industries, including healthcare, transportation, retail, and entertainment. For example, it can be used for medical image analysis, self-driving cars, visual search in e-commerce, and augmented reality in gaming and entertainment.

Chapter 14: Large-Scale Algorithms – Large-scale algorithms are computational methods designed to handle massive amounts of data, such as those generated by modern digital technologies. These algorithms typically involve processing large datasets in parallel or distributed systems and require specialized hardware and software architectures to achieve high performance.

The development of large-scale algorithms has become increasingly important in recent years due to the exponential growth of data generated by various sources such as social media, scientific simulations, and internet of things (IoT) devices. Large-scale algorithms are needed to handle these large and complex datasets efficiently and effectively.

Examples of large-scale algorithms include distributed machine learning algorithms such as Spark MLlib and TensorFlow, graph processing algorithms such as Apache Giraph and GraphX, and parallel processing algorithms such as Hadoop MapReduce and Apache Flink. These algorithms are widely used in various industries, such as finance, healthcare, and social media to analyze large datasets and make data-driven decisions.

Chapter 15: Outlook into the Future: Quantum Machine Learning – Quantum machine learning is an emerging field that combines quantum computing and machine learning. Quantum computing uses the principles of quantum mechanics to perform certain computations much faster than classical computing. Machine learning, on the other hand, involves developing algorithms that can learn patterns and insights from data.

Quantum machine learning aims to leverage the power of quantum computing to develop more efficient algorithms for machine learning tasks, such as classification, clustering, and regression. These algorithms could potentially provide significant speedup and better accuracy compared to classical machine learning algorithms.

There are various approaches to quantum machine learning, including quantum-inspired classical algorithms, quantum-enhanced classical algorithms, and fully quantum algorithms. Some of the challenges in quantum machine learning include designing quantum algorithms that can take advantage of the unique properties of quantum computing, such as superposition and entanglement, and developing hardware and software infrastructure for quantum computing that can support large-scale machine learning tasks.

Quantum machine learning has the potential to revolutionize many industries, including finance, healthcare, and cybersecurity, by providing faster and more accurate predictions and insights from large datasets.

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Chapter 1
Fundamentals

Introduction

This chapter of the book will cover the fundamentals of **artificial intelligence (AI)** and **machine learning (ML)**. We would start by laying out the fundamentals and their definitions to create a common understanding of the field. We will dive into the world of AI and ML by defining the fields and their impact on the world inside and outside of AI. We will as well include the critical concepts and what kind of industry problems could be solved with AI and ML. We will close out the chapter with simple examples to make a differentiation between an AI/ML application and an AI/ML algorithm.

Structure

The chapter covers the following topics:

- Fundamentals of AI and ML
- Defining AI and ML
- History of AI and ML
    - Classic examples of AI and ML
- AI and ML algorithms
    - Examples of AI and ML algorithms
    - Structure of a typical AI and ML algorithm

Objectives

By the end of this chapter, you will gain a comprehensive understanding of AI and ML as general concepts and their underlying fundamentals. Additionally, you will learn about the origins of AI and ML and be exposed to some basic examples. Furthermore, you will grasp the concept of basic data structures associated with these fields.

Fundamentals of AI and ML

The fundamentals of AI and ML encompass a wide range of concepts and techniques. Here are some key fundamentals of AI and ML:

- **Data**: High-quality data is essential for AI and ML. It serves as the foundation for training and evaluating models. Understanding the data, its quality, structure, and representation is crucial for successful AI and ML applications.
- **Algorithms**: Algorithms are mathematical and computational procedures used to solve specific problems or perform tasks. In AI and ML, algorithms are used to train models, make predictions, and make decisions based on data. Examples include decision trees, neural networks, **Support Vector Machines** (**SVM**), and clustering algorithms.
- **Feature engineering**: Feature engineering involves selecting, transforming, and creating relevant features from raw data to improve the performance of ML models. This process helps extract meaningful information and patterns from the data, making it easier for models to learn and make accurate predictions.
- **Model training**: Model training is the process of feeding labeled data into an algorithm or model to learn patterns and relationships. During training, the model adjusts its internal parameters to minimize the difference between predicted and actual outputs. This process often involves optimization techniques, such as gradient descent, to find the best parameter values.
- **Model evaluation**: Evaluating the performance of ML models is crucial to ensure their effectiveness and generalization. Various metrics, such as accuracy, precision, recall, and F1-score, are used to assess the model's predictive capabilities. Cross-validation techniques, such as k-fold cross-validation, help estimate the model's performance on unseen data.
- **Generalization and overfitting**: Generalization refers to a model's ability to perform well on unseen data. Overfitting occurs when a model becomes overly complex and performs well on the training data but fails to generalize to new data. Techniques such as regularization and early stopping are employed to prevent overfitting and promote better generalization.
- **Model deployment**: Deploying ML models involves making them available for use in real-world applications. This includes optimizing the model for efficiency, scalability, and compatibility with the target environment. The model deployment

also involves monitoring the model's performance and retraining or updating it when necessary.

- **Ethics and bias**: As AI and ML systems have a societal impact, understanding the ethical implications and addressing potential biases is crucial. Ensuring fairness, transparency, and accountability in AI systems is an essential consideration. Ethical considerations involve issues such as data privacy, algorithmic bias, and the potential impact of AI on various stakeholders.

These fundamentals provide a solid foundation for understanding and developing AI and ML applications. Mastering these concepts allows practitioners to build robust and effective AI systems. This book will focus on the algorithms that are forming the core of every modern AI and ML application.

Defining AI and ML

Let us now discuss AI and ML in detail.

Artificial Intelligence

Artificial Intelligence is a broad field in computer science that focuses on the creation of systems capable of performing tasks that would typically require human intelligence. This includes tasks like understanding natural language, recognizing patterns, solving problems, learning from experience, and making decisions.

Examples of AI in use today by data scientists include:

- **Natural Language Processing (NLP):** NLP algorithms are used to create systems like *Siri*, *Google Assistant*, and *ChatGPT* (which you currently interact with) that can understand and generate human language.
- **Computer vision**: Algorithms in this domain are designed to interpret and understand the visual world. For instance, Facebook uses computer vision AI to recognize and tag faces in images.
- **Recommendation systems**: Websites like *Amazon* and *Netflix* use AI to recommend products or movies based on a user's past behavior and the behavior of similar users.
- **Predictive analytics**: Many industries use AI to predict future outcomes, like predicting stock prices in finance or disease outbreaks in healthcare.
- **Autonomous vehicles**: Companies like Tesla use AI to enable cars to navigate and understand the world around them.

These examples only scratch the surface of AI's potential. Its reach is continually expanding, making it a crucial tool in a modern data scientist's arsenal.

Machine learning

Machine learning is a subset of AI that gives computers the ability to learn from data and make decisions or predictions without being explicitly programmed to do so. This process involves the development of algorithms that can process large amounts of data, learn patterns within that data, and use this learned information to predict future outcomes or behavior. This *learning* is accomplished by improving the performance of the system over time as it is exposed to more data.

There are three main types of ML, supervised learning, unsupervised learning, and reinforcement learning, which are discussed below:

- **Supervised learning** involves training a model on a labeled dataset, that is, a dataset where the outcome or target variable is known. The model learns the relationship between the features and the target and can then predict the outcome for new, unseen data. For example, a bank might use supervised learning to predict whether a loan applicant will default based on their previous loan history and financial profile.
- **Unsupervised learning** involves training a model on an unlabeled dataset, that is, a dataset where the outcome or target variable is not known. The goal is to discover hidden patterns or intrinsic structures within the data. Common uses include clustering and dimensionality reduction. For example, a retail company might use unsupervised learning to segment its customers into different groups based on their buying behavior.
- **Reinforcement learning** involves training a model to make a series of decisions by rewarding or punishing the model (the *agent*) based on the actions it takes in an environment to reach a goal. The model learns to perform actions that maximize some reward over time. This is often used in robotics, gaming, and navigation. For example, reinforcement learning has been used to train AI to play and win complex games like *Go* and *Chess*.

Modern data scientists need to understand these concepts and techniques to build and deploy effective ML models. Moreover, they often need to use different types of machine learning in concert, depending on the task at hand. They should also be aware of new trends in ML, such as Deep Learning, transfer learning, and active learning, which have led to significant advancements in fields like computer vision, natural language processing, and recommender systems.

History of AI and ML

The development of AI and ML has been an incremental journey spanning several decades. The evolution of these fields has been influenced by various domains like mathematics, statistics, computer science, cognitive psychology, and neuroscience, as discussed in the following points:

- **The 1950s - Birth of AI and ML**: The birth of AI as a distinct field happened during a summer conference at Dartmouth College in 1956, which was attended by pioneers like *John McCarthy*, *Marvin Minsky*, *Allen Newell*, and *Herbert Simon*. Here, they proposed that *every feature of learning or any other feature of intelligence can in principle be so precisely described that a machine can be made to simulate it*.'

  Even before this, in 1950, *Alan Turing* introduced the concept of machine intelligence with the *Turing Test*, a measure of a machine's ability to exhibit intelligent behavior equivalent to, or indistinguishable from, that of a human.

  In 1959, *Arthur Samuel* developed a program that could play checkers and learn from its mistakes, marking one of the first self-learning programs and a seminal moment in ML.

- **The 1960s - Growth and consolidation**: In the 1960s, AI research focused on problem-solving and symbolic methods. AI programs like **DENDRAL** and **ELIZA** were developed during this time.

  ML saw a significant development in 1967 with the creation of the **Nearest Neighbor algorithm**, which started basic pattern recognition.

- **The 1970s - AI Winter and rule-based systems**: The mid-1970s marked the beginning of the first *AI Winter*, a period of disappointment resulting from the overhyping of AI capabilities and subsequent cuts in funding. The focus shifted towards *expert systems* – rule-based systems that tried to mimic the decision-making of human experts.

- **The 1980s – Revival and ML expansion**: In the 1980s, AI saw a revival with the rise of ML. The development of the backpropagation algorithm enabled more efficient training of neural networks, and the advent of SVM led to significant progress in ML.

- **The 1990s – AI and ML Maturity**: The 1990s saw ML mature into a field of its own, with the growth of decision tree algorithms, reinforcement learning, and Bayesian networks. AI and ML began to be used in practical applications, from data mining to industrial robotics.

- **The 2000s - The data boom and rise of deep learning**: The explosion of data in the 2000s, due to the rise of the internet and, later, social media, alongside advancements in computational power and storage, created the perfect conditions for AI and ML to flourish. Deep learning, a subset of ML, started to become feasible, driven by the development of new neural network architectures.

- **The 2010s - AI and ML breakthroughs**: This decade witnessed rapid progress in AI and ML. The development of advanced neural network architectures, like **Convolutional Neural Networks (CNNs)** and **Recurrent Neural Networks (RNNs)**, led to breakthroughs in image and speech recognition and natural language processing.