Artificial Intelligence in Spectroscopy

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TABLE OF CONTENTS

Part III: Artificial Intelligence in Spectroscopy

PREFACE

"Humans should be above. I will order AI to do something and if they don't listen I will gut that AI."
Hideo Kojima (a famous Japanese video game designer)

"In my opinion, «intelligence» means the ability to know or understand an area. If something cannot understand anything, we should not say that it is intelligence, even if it has at least a drop of intelligence."
Richard Stallman (the author of the first software-sharing community)

Dear Reader: an experienced spectroscopist-analyst, a novice researcher, and a student!

Don't be discouraged by these epigraphs. You can continue reading the book and then decide whether you agree or disagree with the opinions of these famous people.

Imagine breaking away from the monotony of everyday work and mentally transporting yourself into a fantasy world where super-intelligent humanoid robots collaborate with computerized spectral devices. These robots are equipped with powerful manipulators for preparing samples.

They analyze data and interpret stunning 3D images created in laboratory space by advanced supercomputers. They push their intellectual limits to unravel the secrets of studied objects and discern their composition.

This scenario may seem like science fiction, but you won't have to wait long for it to become reality. Artificial Intelligence (AI) is rapidly bringing us closer to this dream. However, for now, let's return to the present, turn the pages of this book, and explore what AI truly is. What does it mean for a computer system to utilize AI methods? Can we confidently call it an AI system?

AI is already transforming numerous fields, accomplishing remarkable tasks like computer vision, environmental monitoring, market analysis and decision-making, fraud detection, content moderation, scientific simulations, quality control in food and drug production, healthcare operations, autonomous vehicles, and space exploration. Although computers can tell jokes (provided they've heard them before), humans still hold the upper hand in humor. Nevertheless, don't underestimate AI-it may catch up faster than skeptics think [1, 2].

That said, today's AI systems are still in their infancy. They are the "software kids" - diligent, stunningly successful students [3] who, one day, through an evolutionary process, will be able to transform a network of artificial neurons into a collective superintelligence. Currently, many articles in analytical spectroscopy involve AI-driven research using intelligence algorithms such as clustering, classification, and pattern recognition [3 (and references therein)-7]. Regrettably, the allure of the term "AI" sometimes tempts authors to include it in their article titles unjustifiably, leading to occasional controversy.

This book delves into the foundational principles of AI algorithms, illustrated with numerous examples of spectroscopy applications. It is further enriched with MATLAB programs designed using functional and object-oriented programming paradigms.

The preparation of this book posed significant challenges due to its broad scope. It encompasses the theoretical and technical aspects of processing one- and multi-dimensional signals and tackling applied physicochemical problems in atomic and molecular spectroscopy. Presenting such complex material requires advanced mathematical methods that are often unfamiliar to analytical spectroscopy professionals.

As with our previous books [4, 8-10], the objective is to encourage readers to question the reliability of conclusions and recommendations rather than accepting them without critical examination. Theoretical discussions are complemented by practical examples and simple MATLAB code that non-specialists can adapt to their specific tasks. For those interested in deeper exploration, the book provides opportunities to validate its numerical data through computer simulations. This hands-on approach allows readers to grasp algorithmic details and modify the programs if necessary, ensuring a comprehensive understanding.

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ABOUT THE STRUCTURE OF THE BOOK

The book consists of three parts. The first part, 'Introduction to Artificial Intelligence,' introduces the reader to basic Artificial Intelligence (AI) concepts and answers the question, "Does it mean that a computer system using AI methods is really an AI system?"

The second part introduces AI-based data analytics methods (clustering, data mining, classification, and regression). The author paid special attention to Artificial Networks since this topic is new for spectroscopist-analytics. Numerical examples supplied with Matlab code help the user better understand the operation principles of numerous cumbersome algorithms. This part aims to make it easier to understand the practical methods of AI-based applications to spectroscopy, which is the subject of the following part.

The last part begins with bibliography tables briefly describing hundreds of applications of spectral data analytics methods and related topics in industrial and research laboratories.

For a better understanding of new terminology, Chapter Six, dedicated to the bibliographic analysis of network architecture used in spectroscopy, is placed after some chapters that describe AI-based analytical methods.

We sincerely apologize to all those researchers whose outstanding works were not cited because the book lacks the free space to include a complete bibliography.

The author aimed to give each chapter the status of a self-contained article, whose reading is independent of the other sections. This material presentation allows readers to avoid cramming a previous text before moving on to another topic. The tutorial adjusted MATLAB examples to the goals of each chapter and focused them on the subject.

The programs use open-source spectral databases [1-5].

The book closes with appendices, which include supplementary materials necessary to facilitate the readers' understanding of the theoretical problems discussed in the main text. For example, Appendix B briefly introduces mathematical methods such as singular value decomposition, discrete Fourier transform, and Tikhonov regularization. Reading requires knowledge of secondary school courses on differential calculus, linear algebra, and statistics. To perform the exercises, readers must have programming skills at the middle level of MATLAB and be familiar with the general concepts of object-oriented programming.

For simplicity, the captions of figures, tables, exercises, and expressions have the following structure: "part. chapter-current number."

The author would be very grateful for any criticisms, comments, or proposals regarding this book, which he hopes to consider in his future work.

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ABBREVIATIONS

AI-Artificial Intelligence
AIC-Akaike's Information Criterion
AGL-Agglomerative
AM- Attention Mechanism
ANFIS-Neuro-Fuzzy Inference System
ANN-Artificial Neural Networks (NN)
ANOVA-Analysis of Variance
AR-Association Rules
ARM-AR Mining
BDA-Big Data
BNL-Batch Normalization Layer
BPNN-Back Propagation NN
CA-Cluster Analysis
CAR- Classification Association Rule
CARS-Competitive Adaptive Reweighted Sampling
CF-Cascade Forest
CFT-Continuous FT
CL-Convolutional Layer
CLL-Consistency Level of Link
CLODM-Clustering-based ODM
CLSODM-Classification-based ODM
CNN-Convolutional NN
CPHD-Cophenetic Distance
CWT- Continuous WT
DA-Discriminant Analysis
DALC-Data Analytics Lifecycle
DBSCAN-Density-Based Spatial Clustering of Applications with Noise
DCL-Data Clustering
DCNN- Deep CNN
DCT-Discrete Cosine Transform
DFA - Discriminant Function Analysis
DFT-Discrete FT
DIP-Digital Image Processing
DLCP-Data Lifecycle Process
DM-Data Mining
DSS- Decision Support System
DT- Decision Tree
DTNN- Deep Tensor NN
DW-Data Warehouse
ECOC-Error-Correcting Output Codes
ELM-Extreme Learning Machine
FC-Fully Connected Layer
FCA-Fuzzy Clustering Algorithm
FCOS-Fluorescence Correlation Spectroscopy
FDA-Functional Data Analysis
FFT-Fast FT
FIS-Firefly Interval Selection
FNN- Feedforward NN
Fs-LA-SIBS-Femtosecond Laser-Ablation Spark-Induced Breakdown Spectroscopy.
FT-Fourier Transform
FTIR-Fourier Transform IR
FWHM-Full Peak Width at Half-Maximum
GA-Genetic Algorithm
GALDA-Generative Adversarial Linear DA.
GAN-Generative Adversarial Network
GC-Gas Chromatography
GCN-Graph CNN

GDH-Generalized Discrete Harmonics
GFT- Generalized FT
GenAI-Creative Generation
GenXAI-Explainable Generative AI
GMM-Gaussian Mixture Model
GRNN-Generalized Regression NN
HA-Harmonic Analysis
HC-Hierarchical Clustering
HI-Human Intelligence
HIS-Hyperspectral Imaging
HITL-Human In The Loop
HOOTL-Human Out The Loop
HOTL-Human On The Loop
HPLC- High-Performance LC
HT-Hadamard Transform
ICC-Inconsistency Coefficient
IFT-Inverse FT
IR- Infrared
IR-CF- IR Characteristic Frequencies
IT- Information Theory
KBS-Knowledge-Based Simulation
K-ELM Kernel EML
KM-K-Mean Algorithm
KM-HMR-KM-Hadoop MapReduce
KNN-K-Nearest Neighbor
KPCA-Kernel PCA
LC-Liquid Chromatography
LF-Loss Function
LL-Lazy Learning
LOF-Local Outlier Factor
LR- Logistic Regression
LS-Least Squares
MCD-Monte Carlo Dropout
ML-Machine Learning
MLP-Multilayer Perceptron
MLR-Multiple Linear Regression
MM-Method of Moments
MS-Mass Spectroscopy
MST-Minimum Spanning Tree
NB-Naive Bayes
NIR-Near IR
N-MBL-Non-Linear Memory-Based Learning
NMR-Nuclear Magnetic Resonance
NN-EN-NonNegative Elastic Net
OD-Outlier Detection Method
OLAP-Sophisticated On-Line Analytical Processing
OLS-Ordinary Least Squares
OSC-Orthogonal Signal Correction
PAT- Process Analytical Technology
PC-Principal Component
PCA-PC Analysis
PCR-PC Regression
PLS-Partial LS
PSO- Particle Swarm Optimization
QDA-Quadratic DA
RF- Random Forest
RGB-Red, Green, and Blue
RL-Reinforcement Learning
RNN-Recurrent NN
RS-Raman Spectrum
RSEP-Relative Standard Error of Prediction
RT-Regression Tree
SG-Savitzky-Golay
SFS-Synchronous Fluorescence Spectroscopy
SIMCA-Soft Independent Class Analogy
SL-Supervised Learning
SMF-Softmax Function

SMLR-Stepwise MLR
SMOTE-Synthetic Minority Oversampling
S/N-Signal-to-Noise Ratio
SOM-Self-Organizing (SO) Map
SOFM-SO Feature Maps
SPD-Spectral Databases
SRS-Stimulated Raman Scattering
SV- Silhouette Values
SVD-Singular Value Decomposition
SVM-Support Vector Machine
TMS- Technological Management System
TR-Tikhonov Regularization
UL-Unsupervised Learning
UV-Ultraviolet
VIS-Visible
WM-Waterfall Model
WOA- Whale Optimization Algorithm
WT-Wavelet Transform
XGBoost- eXtreme Tree Boosting System

PART I

INTRODUCTION TO ARTIFICIAL INTELLIGENCE

INTRODUCTION

"-The oldest, shortest words-"yes" and "no"-are those which require the most thought"- Pythagoras [1]

Many years ago, the author of this book, a young man, was profoundly experienced and mentally transported into a fantasy world of robots in the American multimedia franchise Terminator, and he was amazed by Stanisław Lem's fantasy of an intelligent ocean, Solaris. When reading the science fiction novel "The Moon Is a Harsh Mistress" by American writer R. A. Heinlein, it was impossible to imagine that a supercomputer controlling Lunar infrastructure and machinery had achieved self-awareness and developed a sense of humor!

Now, my grandson gives voice instructions to the car's computer about whom to call on the phone and asks questions about a convenient route. Artificial intelligence (AI) programs do all this and many other valuable things that cannot be listed (e.g., computer vision, environment control, market analysis and decision-making, fraud detection, finding potentially harmful content, simulations in scientific research, food and drug production and quality control, healthcare operations, moving cars without a driver, space vehicles without astronauts, and others).

Computers can tell jokes, but only if they have heard them before.

While humans are still better with humor, computers might catch up sooner than skeptics think.

However, generally speaking, they are still "program children" but diligent students, and, over time, maybe in the evolution process, similarly to humans, they will fulfill a fantastic dream by transforming a set of artificial neurons into a collective supermind [2, 3].

Nowadays, numerous articles on analytical spectroscopy are AI-based research that includes Data Analytics algorithms (e.g., clustering, classification, and pattern recognition) [4]. Unfortunately, the impressive AI term sometimes tempts authors to add it to the article's title, although this modification can be controversial.

This part aims to discuss and compare AI vs. human intelligence, which may help to deepen our understanding of the essence of AI and "take down a peg" from some future publications.

The author hopes the reader will answer, "Does it mean a computer system using AI methods is an AI system?" [5].

CHAPTER ONE

PHILOSOPHY OF ARTIFICIAL INTELLIGENCE

The essence and characteristics of intelligence and methods for assessing it have been the subject of centuries-old philosophical discussions [1]. The importance of these problems became especially significant with the emergence of the idea of creating "a thinking machine," the so-called artificial intelligence (AI).

Hundreds of books and thousands of studies are devoted to an in-depth consideration of the problem of AI, the analysis of which goes far beyond the book's scope. Therefore, the author limited himself to a brief introduction to the essence of AI problems, which is essential for a better understanding of the subsequent presentation.

Many engineers and scientists specializing in AI perceive this term as denoting a set of algorithms and ready-made programs that "think" independently with little or no human intervention. In addition, the verb "think," which characterizes humans as the most intelligent form of living organisms, is understood as self-evident. So, before discussing the philosophical problems of AI, think about what intelligence is and how people's intellectual abilities are assessed.

Intelligence

In everyday life, intelligence (from Latin intellectus) is a human ability to learn and solve novel problems in everyday self-maintenance [2].

In a broad sense, intelligence is a cognitive ability that manifests itself in how a person (an agent) perceives, understands, explains, and predicts what is happening, what decisions he makes, and how effectively he acts, primarily in unexpected, unusual situations. Scholastics considered "intelligence" the highest cognitive ability in contrast to elementary abstraction: the outstanding philosophists, I. Kant and further G. W. F. Hegel defined this term as the ability to form metaphysical ideas and reason.

In modern psychology, intelligence is viewed as a complex system of mental operations, specifically information processing. These operations include analysis, synthesis, and generalization. The 'mental speed' at which these operations are carried out is a key indicator of an individual's intelligence level.

The classic definition of intelligence is "Intelligence measures an agent's ability to achieve goals in a wide range of environments" [1]. It is clear that an agent may not only be a human but also an animal, e.g., a cat or parrot. The environment is believed to influence the agent's intellectual abilities, such as learning how to use computers. However, one can argue with this statement.

Really, there are three types of intelligence: 'A' (the biological basis of all cognitive activities of individuals), 'B' (reflects cognitive activities in everyday life, depending on educational, cultural, and socioeconomic factors), and 'C' (psychometric intelligence, measured by tests) [3].

Theories of intelligence [4]

C. Spearman, a pioneer of factor analysis, established the two-factor intelligence theory. He stated that a single g-factor represents an individual's general intelligence across multiple abilities and that a second factor, 's,' refers to an individual's specific ability in one area.

L. Thurstone significantly enriched the understanding of intelligence by expanding on Spearman's two-factor theory and identifying seven primary mental abilities that comprise intelligence.

H. Gardner made a unique contribution to intelligence studies by proposing the concept of multiple intelligences, each representing unique skills and talents, despite the subsequent criticism of his theory.

R. Sternberg integrated components lacking in Gardner's theory: analytical (componential), creative, and practical. They, respectively, characterize abilities to

- analyse problems and arrive at solutions;
- create novel and interesting ideas involving imagination, innovation, and problem solving;
- solve everyday problems by the best fitting between a person and the demands of the environment by adaptation, changing the environment to suit oneself (shaping), or finding a new working environment (selection).

Other theories consider emotional aspects of intelligence, such as problem-solving ability without and with referencing previously acquired knowledge (fluid and crystallized intelligence).

In conclusion, psychologists' different forms of intelligence have dynamic natures; therefore, they overlap and interact.

Article [5] reports models of intelligence, particularly the Cattell-Horn-Carroll one, based on a wide range of cognitive abilities. A network pattern illustrates this model visually.

Intelligence Testing

An essential question immediately arises [6, 7]: "How do you measure intelligence?" Alan Turing, one of the founders of computers, formulated the famous question "Can machines think?" and proposed replacing the intelligence ability "thinking" with a term that we can test [8].

Probably every reader has experienced a headache when testing for admission to a university or a high-tech company. The author of this book recalls with a bashful smile how he received a low grade while answering questions on a geometry test in elementary school.

Let us give simple examples [9].

1) What is the missing number? [0, 1, 1, 2, 3, 5, 8, ?, 21, 34]. Answer: 13
2) Which identical three-letter word, when placed in front of the following words, forms a new word? FUSE, CLAIM, DUCT, CREATE, FIT, FOUND, LONG
   Answer: add PRO to all words
3) One likes 324 but not 323. He likes 2500 but not 2200. He likes 144 but not 145. Which does he like?
   a) 400, b) 401. Clue: One only likes numbers that are perfect squares!

When viewed as a quantifiable attribute, intelligence plays a crucial role in our society. It aids in assessing an individual's capabilities, identifying intellectual disabilities, and projecting their potential in the future.

The IQ test measures the intelligence quotient, which is calculated as (intelligence age / actual age) x 100 in the age or point scale. The first case involves calculating the total points scored in the verbal and non-verbal tests that estimate fluid and crystallized intelligence.

Numerous studies proved that IQ scores have strong construct validity; that is, intelligence tests measure IQ scores indeed (rather than something else), and they are consistent over time (highly reliable)

However, opponents of intelligence testing argue that IQ tests are biased because negative stereotypes about a person’s ethnicity, gender, and age result in lower scores.

The author recommends the open e-book [10] to the interested reader as a bibliographic source for deeper studies.

Classification of AI

Now, let's leave the ongoing discussion between specialists of different profiles about the philosophical problems of the intelligence of living beings and intelligence testing to discuss AI.

Fig. 1.1-1 depicts the classification of AI. Classical AI is based on the assumption that human intelligence is driven entirely by computation; therefore, the computing device can repeat this process. Again, a new question immediately arises: "Can everything be calculated?"

As far as the ultimate laws of nature go, the answer is "no" [11]. However, robots and computers can even recognize (interpret) human emotions by analysing facial expressions and responding accordingly. These calculational facilities are named affective computing [12].

The major components of an AI system are the input device, memory, processing part, and output device.

Just like a brain that does not passively wait for input but is always ready to participate in the action-perception cycle actively, an AI system must interact with the environment by perceiving information through sensors that are responsible for "the cause-and-effect relationship" between symbols manipulated by a computer program and the world. Therefore, without this relationship, classical AI, based solely on the assumption that an appropriately programmed computer is a mind, cannot exist. For example, if a computer that does not understand Hebrew is in a closed room, it will not learn that language from Hebrew input in voice or text form.

The famous 'Rosetta Stone' contained three identical texts carved on it, written in Egyptian hieroglyphs, Egyptian demotic script, and ancient Greek. The Ancient Greeks were well-known to linguists, and comparing the three texts helped decipher the Egyptian hieroglyphs.

Therefore, generally speaking, calculations are only sufficient for understanding when accompanied by additional information [1].

Dear reader! What is your opinion about this remark?

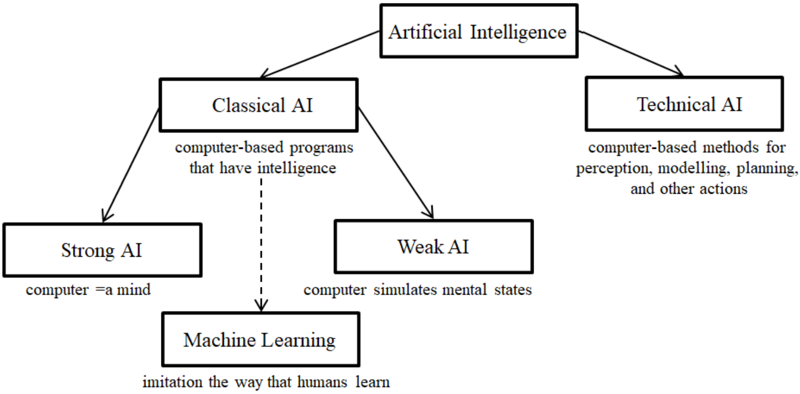

Figure 1.1-1. Types of AI.

So far, we have been discussing AI that mimics human intelligence since humans consider themselves God's cleverest creations. They often rely on a biblical description: "And God said, Let us make man in our image, after our likeness" (Gen. 1:26b)." However, likeness reflects this image in such qualities as goodness, grace, and love. Did God allow us to perfect and clone his creations?

The book [13] raises exciting questions: "Could AI compete with other animals? Maybe there is the most advanced organism whose intelligence we currently understand?"

AI agents are generally considered rational agents. According to decision theory, such an agent perceives the environment, finds options for action, and then makes the best decision to maximize the expected utility.

The agent must remember that its data storage capacity and time resources are limited. Bounded rationality (optimality) means that not only is the best choice essential, but also the resources spent optimizing the choice. In other words, when should the agent stop optimizing and start taking action? [1]. This question is essential for technical AI.

The frame problem means how one can selectively apply relevant knowledge to particular situations to generate practical solutions [14]. Generally, it is "Hamlet's problem: when to stop thinking" [1]. For this goal, classical AI should update the belief system after action without indicating everything that has not changed; this requires specific logic where conclusions may change.

Human intelligence versus AI

The topic of discussion, the differences and similarities between human intelligence (HI) and AI, is of significant importance [1, 15, 16]. This topic is particularly true when considering the fundamental constraints of HI and AI.

The fundamental differences, as outlined in [15], are:

1. Basic structure. HI involves neural "wetware," while now AI is silicon-based intelligence that can be distributed over different digital systems. When learning a new skill, the brain is a biologically isolated system. Drug therapy improves brain function, for example, in dementia, just as increasing memory capacity improves computer efficiency.
2. Signal propagation speed, which decreases from approximately the speed of light in AI systems to the extremely slow conduction velocity of human nerves.
3. Connectivity and communication. People undirectly communicate with each other via language and gestures, whereas AI systems can collaborate using integrated algorithms.

Criticism

There are two forms of communication between humans: verbal and non-verbal [17]. In the first case, style, tone, pitch, and voice volume change how the messages are understood. Non-verbal communication includes sign language, braille (for the visually impaired or who are blind), body language, gestures (hand or arm movements), facial expressions, eye contact, position (how we stand, sit, or hold our arms when we are talking), written communication (e.g., forms of messages).

Is there a program that integrates even a portion of these methods?

4. Updatability and scalability. Unlike HI, updating, upscaling, and reconfiguring AI systems are no problem.
5. Energy consumption. The human brain consumes less energy than a tiny lightbulb in a village. In contrast, a supercomputer with comparable computational performance requires an electricity power station supplied in this village.

Human intelligence's unique properties distinguish it from AI [1].

1. Computers cannot be creative since creativity is not based only on calculations involving acquiring knowledge and technology but should be a gratuitous, unpredictable spark of insight.

   However, new research [18] has challenged this statement, showing that large language models' collective creativity may compete with human creativity (e.g., Hangzhou DeepSeek AI Co).
2. AI has only instrumental (programmed) intelligence about how to achieve goals. It is unclear whether a nonliving system can have "real goals" that require responsibility to achieve them. For example, AI that controls a house ("smart home") is responsible for its normal functioning. It must alarm and try to eliminate the cause of the problem, but what is the punishment of AI if it fails?
3. It is unclear whether AI has a "self" function (become self-aware) that allows moral agency and even patience (a program "patiently" counts until it reaches the limit value of some stopping criterion, for example, the number of iterations a person sets).
4. Human intelligence can operate independently of computers. However, AI cannot autonomously regulate and adapt its functionalities without human intervention (self-management property). For example, indirect human intervention in AI involves creating new data and the knowledge humanity accumulates.

   However, "we are probably not so smart as we think" [15] due to limited cognitive capacity and biases. The last factors are due to distortions of human cognitive information processing that include:

   - Overconfidence is when we believe we're better than we really are, which is contrary to overrating the abilities of others.
   - Availability heuristic, e.g., a witness to a severe road accident caused by a collision with a truck convinces him that all roads are filled with them and that he must be cautious.

A study [16] showed that the accuracy of AI-based and human professorial reviewers in detecting AI-generated medical rephrased articles was close (100% and 96%). However, student reviewers identified only 76% of these articles.

We recommend an exciting continuation of this research [19] to the interested reader.

The review [5] argues the trueness of the statement that "intelligence is not achievement or expertise" with the following definition: "Intelligence is what one does when one does not know what to do." However, numerous AI computer systems demonstrate expertise. Therefore, the reader may see a contradiction in defining the system as AI. The author of this tutorial supposes that a human does not prove intelligence but knowledge in the field of expertise. On the other hand, AI systems mimic human experts. Therefore, they live up to their name.

Exercise 1.1-1

Readers are invited to express their opinions on the issues discussed above and answer these questions:

a. Could an AI computer program pretend to be a student and get an engineering degree (clue [20])?

b. What about biological computers and human microchipping?

The socio-economic benefits of AI are the most critical factor in its integration into our lives.

Table 1.1-1 describes some advantages of AI integration in business.

In recent years, large-scale AI models (foundation models) have significantly expanded the domain of AI [21, 22]. These models allow the generation and adaptation of content across diverse domains, such as creative generations (GenAI).

GenAI means "a shift from AI's ability to "recognize" to its ability to "generate" solutions for a wide range of tasks" [22] as text, images, video, and computer code by identifying specific features in vast volumes of unlabeled and small labeled training data and then reproducing original material that has similar characteristics.

Table 1.1-1. Advantages of AI integration in business (adapted from [21])

Business area	AI integration process
Data expertise	Centralizes data management processes; identifies and maintains high-quality, accessible internal and external data sources, providing security standards and highly controlling access to data, including encryption, monitoring, backup, and recovery.
Business Process	Uses AI-based data and analytics tools to improve productivity by making operational decisions, building a competitive value chain, and automating forecasting beyond reactive reporting.
Workforce	Improves the organization model by creating a strategic change management plan that considers the right capabilities to implement the technology, leverage data, and corresponding business processes and job changes and their impact on the workforce.

Foundation learning expands deep supervised learning to self-supervised plus in-context learning [21].

Explainable Generative AI (GenXAI) is the next stage of GenAI development. The article [21] covers "the nuts and bolts" of GenXAI.

In the limited space of the book, it is impossible to mention even a tiny part of AI's applications in technology, science, and practical life.

We discuss the use of AI in spectroscopy only in Part III.

In the final lines of the chapter, we point out the Knowledge-Based Simulation (KBS) enhanced by AI language in the object-oriented paradigm, which creates behavioral models that answer questions "Beyond What-if...?" [23]. KBS differs from human predictions in that it answers questions in the simple form of "What-if...?"

The outstanding artificial intelligence system successfully used the KBS for molecular spectral analysis [24].

CHAPTER TWO

DOES IT MEAN A COMPUTER SYSTEM USING ARTIFICIAL INTELLIGENCE METHODS IS REALLY AN ARTIFICIAL INTELLIGENCE SYSTEM?

According to the classical definition, "Intelligence is a measure of a person's ability to perceive, understand, explain, and predict what is happening and the effectiveness of his decision-making, primarily in unexpected, unusual situations" [1]. In other words, "Intelligence is what one does when one does not know what to do."

Bibliographical analysis shows that so-called AI-based computer systems often perform priory-predefined tasks and know what to do. For example, modern systems that recognize unknown persons using databases of photographs or fingerprints have replaced professional police experts who successfully revealed criminals manually with paper card files of their fingerprints more than a hundred years ago. The review questions the accuracy of the statement that "intelligence is not achievement or expertise." According to this conclusion, the above systems are not indeed AI. However, they mimic the intellectual actions of humans [1].

Let us expand this definition: "AI systems mimic the intellectual actions of humans aimed to achieve the apriori-defined goal using experience accumulated in the supervised learning controlled by humans and self-learning." Therefore, in this sense, they might belong to AI and live up to their name.

However, isn't counting an intellectual activity? Generally speaking, an intellectual activity must involve learning or thinking. A regular calculator, performing all actions according to the embedded program, does not learn anything new and think. It could be considered an AI system. The author leaves it to the reader to discuss this philosophical problem [1].

Many publications use the terms Machine Learning (ML) and Deep Learning (DL) as essential components of AI and often do not distinguish between them. According to [2], Machine Learning (ML) is a specific technological group of AI, which includes many technologies, one of them being DL.

ML is a self-learning modelling technique that analyses the training data and finds the model by itself, thus replacing humans. The chain

$$Training\ Data -> ML -> Data\ Model \qquad (1.2-1)$$

represents the learning process.

Unfortunately, standard physical or logical laws-based modeling is not a panacea. For example, pure mathematical analysis of speech using discrete transforms [3] is impossible due to language accents, which cause the complex overtone pattern of people's voices. Therefore, a learning process is needed.

Similarly to supervised data analytics [4], a critical problem of ML is selecting a training set that properly reflects the data being processed. The "universal" or "general" ML model, which produces results independent of the training or input data set, is a pipe dream.

The generalization process may lead to overfitting. For example, the tendency to divide a group of points into clusters may generate unreal boundaries (Fig. 1.2-1a), just like the "more precise" smoothing of the straight line with the high-order polynomial produces a "serpentine" curve (Fig.1.2-1).

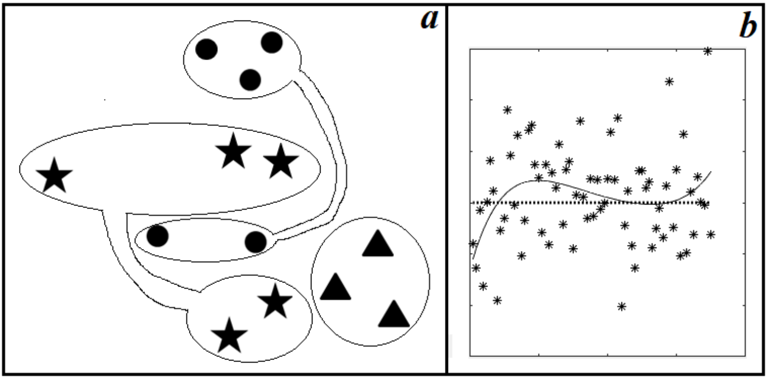

Figure 1.2-1. Overfitting. (a) Clustering. (b) Smoothing the horizontal line (dotted curve) with noise (asterisks) by the fifth-order polynomial (solid line).

Regularization solves the last problem by compromising between the smoothness of the approximated curve and its closeness to the original data [5]. Appendix B2 considers the first case.

There are three types of ML:

- Supervised learning (SL).
  SL learns from training data tagged with a correct answer or classification. SL needs a supervisor as a teacher. The process is repeated to revise a model to reduce the difference between the correct output and the model output for the same input. A perfectly trained model will produce a correct output corresponding to the input of training data. Classification and regression belong to SL.
- Unsupervised learning (UL).
  Analysis of input data properties and preprocessing involves UL; therefore, the training set contains only inputs that do not have correct outputs. A typical example of UL is clustering (Chapter 2.2).
- Reinforcement learning (RL).
  Control and game plays that require optimal interaction use RL. This topic is out of the tutorial.

Nowadays, numerous articles on Analytical Spectroscopy are AI-based research that includes Data Analytics algorithms (e.g., clustering, classification, pattern recognition) [4]. Unfortunately, the impressive AI term sometimes tempts authors to add it to the article's title, although this modification can be controversial.

Data Analytics [4], as the conductor of the analytical 'Big Band' in spectroscopy [6], illustrates how smart computerized methods simulate the "invisible" simple human processing in mind (Table 1.2-1). Moreover, the consumer often takes human actions, which are the core of the AI algorithms, for granted.

This statement becomes more apparent from Table 1.2-1, which emphasizes human involvement in developing, training, and operating AI systems.

The main features of HITL (Human-In-The-Loop) are [7]:

- *Deep learning.* A human examines AI examples with low prediction confidence and presents them for annotation or labeling. The AI model learns continuously and enhances its accuracy.
- *Human oversight.* A human expert reviews and verifies AI systems' outputs or recommendations before any real-world action is taken.
- *Human in the loop control.* Humans adjust the AI system’s behavior or modify its output in real time.
- *Collective intelligence*. The symbiosis between humans and AI systems interactively facilitates a collaborative process. Humans provide training data, refine results, and help AI understand the larger context.