ISBN: 978-81-979987-5-1

INNOVATIVE APPROACHES IN SCIENCE AND TECHNOLOGY RESEARCH

VOLUME I

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Bhumi Publishing, India
First Edition: October 2024

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Published by:

Bhumi Publishing

BHUMI PUBLISHING

Nigave Khalasa, Tal – Karveer, Dist – Kolhapur, Maharashtra, INDIA 416 207

E-mail: bhumipublishing@gmail.com

PREFACE

Science and technology have always played pivotal roles in the advancement of human civilization. As we move deeper into the 21st century, innovation within these fields is accelerating at an unprecedented pace. The ability to integrate new techniques, methodologies, and interdisciplinary approaches has become essential for pushing the boundaries of knowledge and solving complex global challenges. This book, Innovative Approaches in Science and Technology Research, highlights some of the most groundbreaking advancements that reflect the transformative power of modern science and technology.

In today's era, research is no longer confined by traditional boundaries. From biotechnology and nanotechnology to advanced computing and materials science, the convergence of disciplines is leading to a renaissance in research and development. This volume showcases the innovative approaches being employed across a variety of scientific fields, emphasizing the importance of creativity and collaboration in driving forward research that can address real-world problems. By exploring these cutting-edge methodologies, we aim to inspire both current and future researchers to think beyond conventional paradigms and embrace new techniques that can yield transformative results.

The chapters in this book cover a diverse range of topics, each contributing to the overarching theme of innovation. Whether it's harnessing the power of artificial intelligence for data analysis, employing nanomaterials for environmental applications, or advancing the understanding of biological systems through molecular techniques, the research presented here demonstrates how novel approaches are reshaping the landscape of science and technology.

We hope this book serves as both an inspiration and a resource for scientists, engineers, and technologists, encouraging them to adopt innovative approaches in their own work. By embracing the spirit of innovation, we can collectively unlock new possibilities and create a brighter, more advanced future for all.

Editors

TABLE OF CONTENT

Innovative Approaches in Science and Technology Research Volume I
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REVIEW OF FIRST ORDER DIFFERENTIAL EQUATION AND ITS APPLICATIONS

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1. Introduction:

We live in a world of interrelated changing entities. The position of earth changes with time, the velocity of a falling body changes with distance, the area of circle changes with radius etc. In the language of mathematics, changing entities are called variables and the rate of change of one variable with respect to another is called derivative. Equations which express a relationship among these variables and their derivatives is called differential equation. Differential equation is very important in engineering, physics, economics and many areas of science and technology. In this chapter we will define first order first degree differential equation. Then we shall study some special types of first order differential equations such as Separable equations, Homogeneous equations and their solutions with the help of examples. And finally, the orthogonal trajectories which are applications of above-mentioned differential equations.

2. The Differential Equation

2.1 Definition:

An equation involving one dependent variable and its derivatives with respect to one or more independent variables is called a differential equation.

2.2 Definition:

The differential equation in which dependent variable depends only on one independent variable is called an ordinary differential equation.

2.3 Definition:

The order of a differential equation is the order of the highest order derivative involved in the equation.

2.4 Definition:

The degree of a differential equation is the highest power of highest ordered derivative involved in the equation after clearing all radical and fractions, if they exist.

2.5 Definition:

The first order and first degree differential equation is an equation of the form $F\left(x, y, \frac{dy}{dx}\right) = 0$. It may also be expressed as $\frac{dy}{dx} = f(x, y)$ or $Mdx + Ndy = 0$ where $M = M(x, y)$ and $N = N(x, y)$ are functions of x and y.

3. Separable Differential Equation.

In this type of equation, we can separate the variables x and y in such way that the coefficient of dx is a function of x alone or constant and the coefficient of dy is a function of y alone or constant.

Thus, the equation may be written as $M(x)dx = N(y)dy$ or $\frac{dy}{dx} = \frac{M(x)}{N(y)}$ where M and N are functions of x and y respectively.

The solution of this differential equation is given by the equation $\int M(x)dx = \int N(y)dy + C$, where C is constant of integration.

3.1 Example: Solve $\frac{dy}{dx} = xy + y + x + 1$.

Solution: We can write the above differential as

$$\frac{dy}{dx} = y(x+1) + (x+1)$$

$$= (y+1)(x+1)$$

$$\therefore \frac{dy}{(y+1)} = (x+1)dx$$

Therefore, solution of above differential equation is,

$$\int \frac{1}{(y+1)} dy = \int (x+1)\, dx + C$$

$$\Rightarrow \log|y+1| = \frac{x^2}{2} + x + C.$$

3.2 Example: Solve $\frac{dy}{dx} = \frac{-3e^x \tan y}{(1-e^x)\sec^2 y}$.

Solution: We can write the above differential as

$$(1-e^x)\sec^2 y\, dy + 3e^x \tan y\, dx = 0$$

$$3\frac{e^x}{1-e^x}dx + \frac{\sec^2 y}{\tan y}dy = 0$$

$$\therefore\ 3\int \frac{e^x}{1-e^x}dx + \int \frac{\sec^2 y}{\tan y}dy = 0$$

$$\therefore\ -3\log(1-e^x) + \log\tan y\ = \log C$$

$$\therefore \qquad \log\tan y = \log C + 3\log(1-e^x)$$

$$\therefore \qquad \log\tan y = \log C + \log(1-e^x)^3$$

$$\therefore \qquad \log\tan y = \log C(1-e^x)^3$$

$\therefore \quad \log \tan y = \log C(1-e^x)^3$

$\therefore \quad \tan y = C(1-e^x)^3$ is required solution.

4. Homogeneous Differential Equation.

A differential equation of first order and first degree is said to be homogeneous if it can be put in the form $\frac{dy}{dx} = f\left(\frac{y}{x}\right)$.

The homogeneous differential equation can be reduced to a variable separable form by substituting $\frac{y}{x} = v$, i.e., $y = vx$.

$\therefore \frac{dy}{dx} = v + x\frac{dv}{dx}$ i.e. $v + x\frac{dv}{dx} = f(v) \Rightarrow \frac{dv}{f(v)-v} = \frac{1}{x}dx$.

Thus, the general solution is given by $\int \frac{1}{f(v)-v}dv = \int \frac{1}{x}dx + C$, where C is integrating constant.

4.1 Example: Solve $(x^3 + 3xy^2)dx + (y^3 + 3x^2y)dy = 0$.

Solution: Given $\frac{dy}{dx} = -\frac{x^3+3xy^2}{y^3+3x^2y} = -\frac{1+3\left(\frac{y}{x}\right)^2}{\left(\frac{y}{x}\right)^3+3\left(\frac{y}{x}\right)}$

Put $\frac{y}{x} = v$ i.e., $y = vx \Rightarrow \frac{dy}{dx} = v + x\frac{dv}{dx}$

$\therefore \; v + x\frac{dv}{dx} = -\frac{1+3v^2}{v^3+3v}$

$\therefore \; x\frac{dv}{dx} = -\frac{v^4+6v^2+1}{v^3+3v}$

$\Rightarrow \; 4\frac{dx}{x} = -\frac{4v^4+12v}{v^4+6v^2+1}$

On integrating, $4\log x = -\log(v^4 + 6v^2 + 1) + \log C$

$\Rightarrow \log x^4 = \log\left[\frac{C}{v^4+6v^2+1}\right]$

$\Rightarrow x^4(v^4 + 6v^2 + 1) = C$

$\Rightarrow y^4 + 6x^2y^2 + x^4 = C$ as $\frac{y}{x} = v$, is the solution.

4.2 Example: Solve $\frac{dy}{dx} = \frac{y}{x} + tan\left(\frac{y}{x}\right)$.

Solution: Put $\frac{y}{x} = v$ i.e., $y = vx \Rightarrow \frac{dy}{dx} = v + x\frac{dv}{dx}$

$\therefore \; v + x\frac{dv}{dx} = v + \tan v$

$\Rightarrow \frac{dx}{x} = \frac{\cos v}{\sin v}dv$

On integrating, $\log x + \log C = \log \sin v$

$\Rightarrow \; xc = \sin v$

$\Rightarrow \; xc = \sin\left(\frac{y}{x}\right)$ as $\frac{y}{x} = v$, is the solution.

5. Orthogonal Trajectories.

5.1 Definition:

A curve which cuts every member of a given family of curves in accordance with some given law is called trajectory of the given family of curves. And if a curve cuts every member of given family of curves at right angles, it is called an orthogonal trajectory.

5.2 Determination of orthogonal trajectories:

Let the equation of the given family of curves be $f(x, y, c) = 0$ where c is a parameter.

Differentiating with respect to x and eliminating c, we shall arrive at the differential equation of the given family of curves $f\left(x, y, \frac{dy}{dx}\right) = 0$. Next, we replace slope $\frac{dy}{dx}$ of family $f(x, y, c) = 0$ by $-\frac{dx}{dy}$ to obtain the differential equation of the orthogonal trajectories, and finally, solve this new differential equation.

5.3 Example: Find orthogonal trajectories of $x^2 + y^2 = c^2$.

Solution: Given equation of family of circles is

$x^2 + y^2 = c^2$.

On differentiation with respect to x, we get

$2x + 2y\frac{dy}{dx} = 0$ i.e., $x + y\frac{dy}{dx} = 0$

now replace the slope $\frac{dy}{dx}$ by $-\frac{dx}{dy}$.

$\therefore\ x + y\left(-\frac{dx}{dy}\right) = 0\ \Rightarrow\ \frac{dy}{y} = \frac{dx}{x}$

On integrating, $\log y = \log x + \log c$

$\Rightarrow\ y = cx$ which is required orthogonal family of curves.

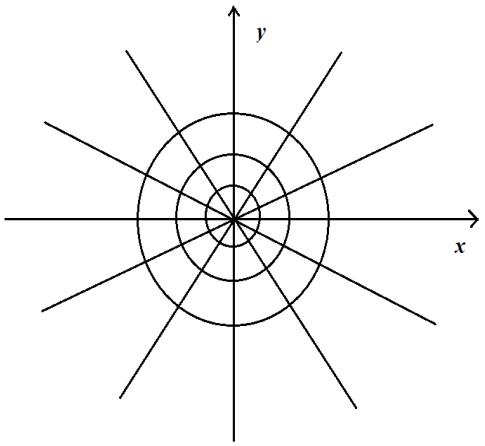

Figure 1

In figure 1, circles are given family of curves and doted straight line are family of orthogonal curves.

5.4 Example: Find orthogonal trajectories of $x^2 + y^2 = 2cx$.

Solution: Given equation of family of circles is $x^2 + y^2 = 2cx$.

On differentiation with respect to x, we get $2x + 2y\frac{dy}{dx} = 2c$ i.e., $x + y\frac{dy}{dx} = c$.

Eliminating c using above two equations, we get

$\frac{dy}{dx} = \frac{y^2 - x^2}{2xy}$.

now replace the slope $\frac{dy}{dx}$ by $-\frac{dx}{dy}$,

we have $\frac{dy}{dx} = \frac{2xy}{x^2-y^2} = \frac{2\left(\frac{y}{x}\right)}{1-\left(\frac{y}{x}\right)^2}$ which is homogeneous equation.

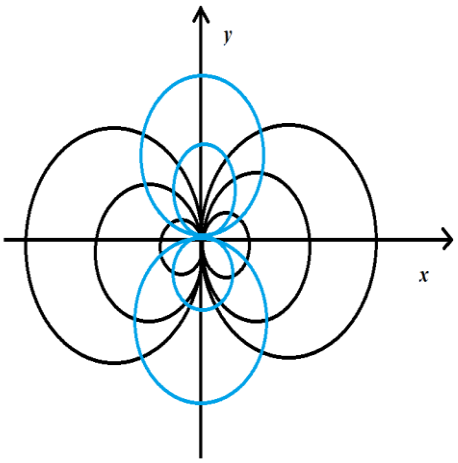

Figure 2

Put $\frac{y}{x} = v$ i.e., $y = vx \Rightarrow \frac{dy}{dx} = v + x\frac{dv}{dx}$

$\therefore\ v + x\frac{dv}{dx} = \frac{2v}{1-v^2} \Rightarrow x\frac{dv}{dx} = \frac{2v}{1-v^2} - v$

$\Rightarrow \frac{dx}{x} = \frac{1-v^2}{v(1+v^2)}$

$\Rightarrow \frac{dx}{x} = \left(\frac{1}{v} - \frac{2v}{1+v^2}\right)dv$, on resolving into partial fractions.

$\Rightarrow \log x = \log v - \log(1+v^2) + \log c$

$$\Rightarrow x = \frac{cv}{1+v^2}$$

$\Rightarrow x\left(1+\frac{y^2}{x^2}\right) = c\left(\frac{y}{x}\right)$, as $\frac{y}{x} = v$

$\Rightarrow x^2 + y^2 = cy$, which is required orthogonal family of curves, c being parameter.

In figure 2, circles whose center point lies on x- axis are given family of curves and circles those center point lies on y- axis are family of orthogonal curves.

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HYBRID AMPHIPHILIC PEPTIDO- FOLDAMER FOR GENE DELIVERY

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Introduction:

Bio-macromolecules, mainly proteins and nucleic acids adopt specific structure (conformation) that are responsible for their various bio functions. During the translation process proteins started to fold into a unique 3-dimentional shape, the "native state" in which they gain functionality. A correct folding pattern is important because it generates "active sites" in which functional groups are often widely spaced along the protein primary sequence. Understanding the close relationship between structure and activity as well as the principles that govern the correct folding pathway of the backbone may allow the *de novo* design of biomimetic polymers. Such syntheses can have important practical applications in pharmaceutical and material science. This represents the research field of "Foldamers". A foldamer is defined as an oligomer that adopts a well-defined conformation stabilised by non-covalent interactions between non-adjucent residues in solution.[1]

In the past decades, many groups have devoted their research to the design and synthesis of a variety of monomers and their corresponding foldamers.[1] According to the nature of their units, all these oligomers can be grouped into two main classes: "Aliphatic" foldamers, which have saturated carbon chains separating amide or urea groups (Figure 1). Example of this group include the β[1f]-, γ[1h]-, δ[1i]-, oligourea[1j], azapeptides[1k], pyrrolinones[1l], α-aminoxy peptides[1m] and sugar-based peptides[1n]. The second class makes use of aromatic spacers within the backbone (Figure 1).[1o]

Keywords: Non-Viral Delivery System, Chemical Delivery System, Peptide, Secondary Structure, Foldamer, Gene Transfection, Gene Therapy

The initial monomer selection is typically affected by a variety of factors including the ease of their synthesis, structural characterisation, basic units should be amenable to design and modify to achieve specific needs and the scaffold should exhibit a controlled rate of biodegradation of the material. However, most of the above-mentioned criteria used in foldamer design have been largely developed with peptides composed of α- amino acids,

which leads to the question of whether our understanding is overly parameterized and specific to conventional peptide, or whether it is truly molecular in nature.

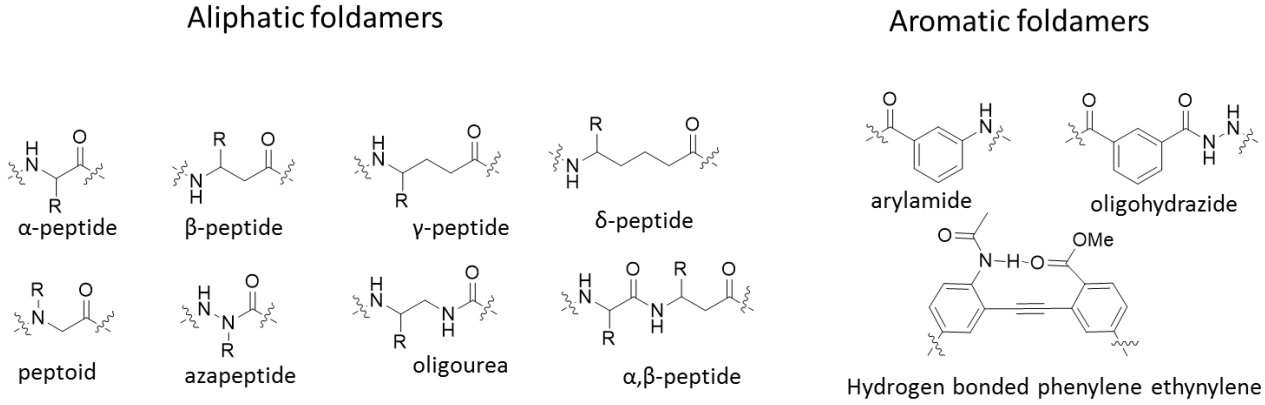

Figure 1: Examples of foldamer frameworks

To address this question, it is important to extend the system by using synthetic building blocks and molecular framework for the design of hybrid peptide composed of homo and hetero oligomers of α, β and γ amino acids in their backbone. The hybrid peptide possess higher proteolytic stability compare to their α-residues which may lead to their higher degree of biological application such as ligand enzyme interaction, ligand receptor interaction, biosensor etc. The insertion of an additional carbon atom into the polypeptide backbone enhances the conformational versatility of these residues. Recent studies established that monosubstituted γ- and β- amino acid support the formation of folded helical structures to a substantially greater extent than their α- amino acid counterpart.[1,2] Thus, proteolytically more stable hybrid peptide with the tendency to fold into tubular or helical conformation with functionalities projected in a convergent manner to form cavity like moieties where small molecules or ions can bind and provide a great opportunity for the design of foldamer receptor for molecular recognition. In this manner, molecular recognition of biomacromolecules such as proteins and DNA by using folded peptide provided a potent therapeutic, pharmaceutic and drug discovery platform for various disease including cancer and infection.[3] In this type of recognition, the target is usually larger than the receptor molecule. The foldamer is often designed to project functionality in an ordered fashion that will complement the surface of the desired target. Thus, gene i.e. DNA or RNA has a high-negatively charged ribophosphate backbone that can be readily targeted by polycationic foldamer compounds. Polycationic foldamers that can bind DNA/RNA and transport them across the cell membrane into the cell may serve as gene delivery vectors for gene therapy either by rectifying a missing or defective gene or to

express a protein of therapeutic interest.[4,5] Due to the sensitivity of DNA/RNA to the nuclease of the biological medium, the hydrophilic poly anionic nature of the DNA/RNA macromolecules and their large size prevent penetrating passively through the cell membrane. Therefore gene (DNA/RNA) must be associated with the delivery system or vector that carries the therapeutic gene, protecting from degradation by nuclease and making sure that it can efficiently translocate inside the cell through attachment to the target cells, cell membrane passage, escape from the endolysosome to reach into the cytosol, and, if possible, transport to the nucleus for the expression of the desired protein (Figure 2 shown the mechanistic pathway of gene delivery). The carriers are generally classified into two groups viral and non-viral. For instance, viral carriers have higher transfection efficiency but can be cytotoxic, may elicit an immune response or can be integrated into the host chromosome. Cationic lipids, polymers, dendrimers and peptides are the most common non-viral vectors.[6] However, lipids vectors, cationic polymer or dendrimer have several drawbacks of being highly toxic for in vivo applications as well as the low transfection efficiencies of non-viral carriers limited their clinical applications.

Although there are several reported non-viral vectors in the literature (lipid, polymer and dendrimers vector) but very less attention has paid to peptidomimetic foldamers vectors composed of homo and hetero oligomers of α-, β- and γ- amino acids in their backbone as a gene carrier. In addition, a deeper exploration of their secondary structure and relation between structure and function will provide a better understanding of their bio-functional behaviour which may assist in developing foldamer based new drugs and materials. These considerations have offers a myriad of opportunities for design of peptidomimetic foldamers, their conformational study and their applications as gene delivery vector. In this chapter highlighted the design principle of peptido-foldamer composed with α, β and γ amino acids in their backbone and their application in gene delivery purpose.

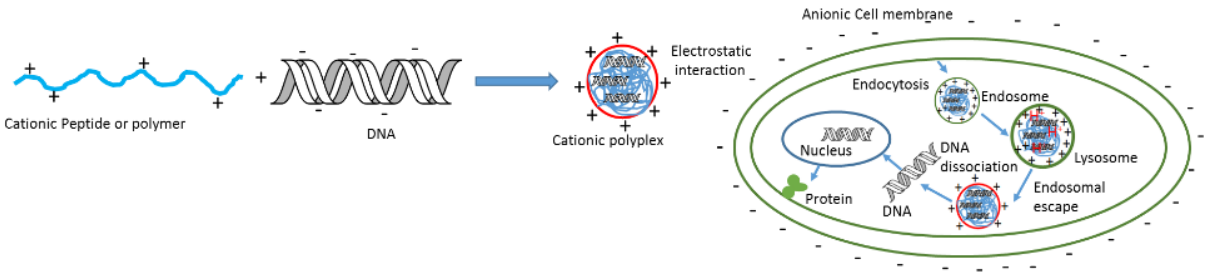

Figure 2: The schematic presentation of gene delivery process of cationic peptide or polymers

Benefit of using peptide foldamer as gene delivery vector

In an attempt to expand the existing pool of peptide as gene vector we are interested in generating hybrid amphiphilic peptides consisting of α, β and γ amino acid as hydrophobic residues and charged amino acids such as lysine, arginine, and histidine as hydrophilic residues. Because of amphiphilic nature of cell membrane, it is important the presence of polar and non-polar faces of a secondary structure of peptide foldamer. To approach the gene delivery into a cell the foldamer vector must first pass through the outer membrane which is composed of phospholipid bilayer (Barrel Stave model). In this mechanism, the amphiphilic conformation of folded peptide plays a central role in which the hydrophobic surfaces of peptide interact with the lipid chains of the membrane core while the cationic hydrophilic surface form the central lumen of the channel. Thus amphiphilic conformation is required in foldamer backbone for cellular uptake purpose. X-ray diffraction studies of peptides have made a possible detailed understanding of the conformational properties of amino acids containing peptide sequences.

Design principle of peptide foldamer

The proposed project is based on the observation that β- and γ- amino acid residues derived from the homologation of α-amino acid have significantly greater tendency to fold into a helical conformation as compare to their α-amino acid counterpart.[1,2] There are currently a great deal of interest in the area of peptidomimetic foldamer with hybrid backbone containing α, β and γ- amino acids. This interest is a consequence of the observation of diverse intramolecularly hydrogen bonded structure in hybrid peptides. The effect of substitution on the conformations of β- and γ- peptides adopt helical structures required by gauche conformation about the θ torsion angles defined by Cα-Cβ and Cα-Cβ, Cβ-Cγ bond, respectively (Figure 3a).

It is proposed to synthesize several β- and γ- analogues of hydrophobic α-amino acid such as Ala, Val, Leu, lle, Phe etc. through homologation of α-amino acid to permit incorporation into design peptide sequences by both solution and solid phase. With the use of cationic amino acid residues such as Lys, Arg, His etc. in hybrid peptide sequences, it is possible to generate amphiphilic helical conformation with cationic side chain which may have high potential to bind with DNA/RNA through electrostatic and hydrophobic interactions (Figure 3b, probable peptide sequence composed of hydrophobic αβγ amino acid of Val and Arg, Lys as hydrophilic part). Thereby, presenting an attractive opportunity for the design of cationic hybrid peptides, their conformational analysis, binding with

DNA/RNA and delivery into the cell will be an important focus of this project. The details study of peptide-DNA complex formation in a sequence and structure specific manner will also be investigated by using various technique such as ITC, UV-Vis and DLS etc. and finally in vitro study by using various cell line will be performed.

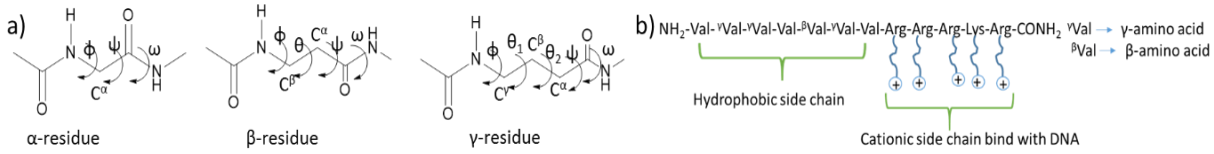

Figure 3. a) Definition for the torsional angles in α-peptide, β-peptide and γ peptide. b) Hybrid peptide sequence composed of hydrophobic αβγ amino acid of Val and Arg, Lys as hydrophilic part, cationic side chain will bind with DNA.

Methodology

Amino acid and peptide synthesis

i. Synthesis of conformationally constrained β and γ amino acid: Numerous procedures are available in literature for the synthesis of β-amino acids based on Arndt-Eistert homologation[7] and γ-amino acids based on the preparation of primary amines, for example by (1) Curtious rearrangement of cycloalkane diacetic acid monoester, (2) 'Hofmann' rearrangement of cycloalkane diacetic acid monoamide or Lossen rearrangement.[8] N-Boc protected 1-aminomethylcyclohexane carboxylic acid was prepared according to literature procedure followed by Fleming *et al*.[9] We are interested in synthesizing αβγ-hybrid peptide backbone by incorporating β- and γ-amino acid as hydrophobic constrained amino acid residues and lysine, arginine, histidine as a hydrophilic amino acid residues.

ii. Synthesis of N-protected amino acids using tert-butyloxycarbonyl (Boc). iii. Coupling mediated by dicyclohexylcarbodiimide/1-hydroxybenzotriazole (DCC/ HOBT). iv. Deprotection of Boc group using 98% HCOOH. v. Solution phase and solid phase synthesis of αβγ-hybrid peptides. vi. Purification of peptides using Column Chromatography and HPLC. vii. Characterisation of peptides using ^{1}H NMR, ESI-MS and MALDI-TOF.

Conformational study of peptides

i. Solution Phase Conformational analysis using Two – Dimensional NMR Spectroscopy.

ii. Crystal structure determination using X-Ray diffraction. iii. Conformational stability using Circular Dichroism.

Peptide-DNA/RNA complx

i. Study of Peptide-DNA/RNA complex formation by using UV-Vis, emission spectroscopy, DLS, ITC and various electronic microscopic image (AFM, TEM).
ii. In vitro delivery of DNA/RNA by using various cell line will be performed.

Conclusion:

Gene therapy has become a promising strategy for treating many diseases such as cancer, AIDS, cardiovascular disease etc. However, the main challenge facing gene therapy which prevents its widespread application in vivo is to find efficient delivery system capable of protecting and delivery gene (DNA/RNA) to target cells in which it can successfully express and also to decrease the side effects of delivery system. This led researchers to design new cationic amphiphilic peptidomimetic foldamer as a delivery system. Due to their higher proteolytic stability, biodegradability, less cytotoxicity may allow them as superior gene delivery system. For successfully gene delivery the following steps can be followed such as:

1) synthesis and characterisation of β-and γ-amino acid from α-amino acid;
2) synthesis of series of hybrid peptide sequences both in solution and solid phase.

Moreover, on basis of initial results as well as for details understanding between structure and function, further modification of peptide sequence will be done which may assist in developing new drugs and pharmaceutical agents.

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SECURING THE DIGITAL FRONTIER: CYBERSECURITY SOLUTIONS FOR MODERN BANKING

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Abstract:

The rapid growth of digital banking has revolutionized the financial sector, offering unprecedented convenience and accessibility for consumers. However, this transformation has also introduced significant cybersecurity challenges, as banks face increasing threats from cybercriminals seeking to exploit vulnerabilities in digital infrastructure. This chapter delves into the critical role of cybersecurity in protecting digital banking systems, focusing on safeguarding sensitive financial data, preventing fraud, and ensuring regulatory compliance. It explores key security measures, including encryption, multi-factor authentication, biometrics, and network security protocols designed to protect online transactions and customer information. The chapter also addresses emerging threats such as phishing, ransomware, and identity theft, along with the integration of artificial intelligence (AI) and machine learning (ML) to enhance threat detection and response in digital banking environments. As digital banking continues to evolve, the chapter highlights the importance of proactive cybersecurity strategies to build trust, safeguard assets, and maintain the resilience of modern financial institutions in the face of ever-evolving cyber threats.

Keywords: Digital Banking, Cybersecurity, Artificial Intelligence, Machine Learning

Introduction:

Digital banking encompasses the complete digitization of traditional banking services, allowing customers to conduct transactions online or through mobile apps anytime and anywhere. It offers a range of services, including account management, fund transfers, loans, and customer support, all designed for user convenience. Digital banking faces several significant challenges that can impact its effectiveness and growth.

One of the most pressing issues is cybersecurity threats, with increasing incidents of phishing and ransomware attacks jeopardizing customer data and trust [1]. Additionally, regulatory compliance presents a complex landscape; banks must navigate various laws

related to data protection and anti-money laundering, which can be both challenging and costly [2]. The digital divide further complicates matters, as ensuring access to digital banking services for underserved populations, particularly in rural areas, remains a critical concern [3]. Moreover, many banks grapple with technology integration, as legacy systems may struggle to work seamlessly with newer technologies, hindering innovation [4].

Lastly, gaining customer trust and adoption is essential, as many consumers still prefer traditional banking methods due to concerns about security and usability, making it crucial for digital banks to demonstrate reliability and ease of use [5].

Some of the cyberattacks that happened in India are listed here.

(i)HDFC Bank (India) - Cyber Attack Incident (2020)

According to The Economic Times article HDFC Bank faces service disruptions due to cyberattack. In December 2020, HDFC Bank faced a cyberattack that caused service disruptions, affecting its mobile banking and internet banking services. Customers experienced difficulties in accessing their accounts, leading to frustration and trust issues. The bank had to reassure customers and implement additional security measures[6].

(ii) SBI Card - Data Breach (2020)

In May 2020, a data breach affecting SBI Card was reported, where sensitive customer data, including names, phone numbers, and card details, was exposed on the dark web. The breach raised concerns about the bank's data security practices, leading to increased scrutiny and customer concerns over privacy[7].

(iii) Australian Banks - Phishing Scams (2020)

Major Australian banks reported an increase in phishing scams targeting their customers, with scammers impersonating bank officials to steal credentials. The incidents led banks to launch awareness campaigns to educate customers about recognizing and reporting phishing attempts[8].

Cybersecurity in digital banking

Cybersecurity is essential in digital banking due to the need to protect sensitive customer data, maintain trust, and ensure compliance with regulatory requirements. Digital banking platforms manage vast amounts of personal and financial information, making them prime targets for cybercriminals. A breach of this data can result in identity theft, fraud, and significant financial losses for both customers and financial institutions.

Robust cybersecurity measures are critical for safeguarding the confidentiality and integrity of this information, which, in turn, helps build and maintain customer trust. Trust

is the cornerstone of the banking industry, and any compromise in security can severely damage a bank's reputation, leading to customer attrition and loss of business

Literature review

Artificial Intelligence (AI) encompasses a variety of techniques aimed at replicating complex abilities, such as making autonomous decisions and using language[9] (Truby, Brown, and Dahdal 2020). Within this realm, Machine Learning (ML) focuses on identifying patterns in data to make informed decisions. ML is categorized into two types: supervised learning, where the system receives explicit correct answers, and unsupervised learning, where it does not [10].

AI and ML can also enhance threat intelligence by analyzing data from multiple sources to identify emerging threats. Predictive analytics can help banks anticipate cyber threats and take proactive measures. Research emphasizes the role of AI in predicting potential cyberattacks based on historical data and current threat landscapes[11].

AI and ML are increasingly being leveraged in cybersecurity to detect and respond to threats in real time. Machine learning algorithms can analyze vast amounts of data to identify patterns and anomalies that may indicate fraudulent activity. A study demonstrates that ML techniques[12], such as anomaly detection and supervised learning, can effectively predict and identify potential security breaches in digital banking systems.

Despite the advantages, the implementation of AI and ML in cybersecurity presents challenges, such as data privacy concerns, algorithmic bias, and the need for transparency. A study discusses the ethical implications of using AI in decision-making processes and highlights the importance of maintaining user trust while implementing AI solutions[13].

As digital banking continues to grow, so does the sophistication of cyberattacks. According to a report by the World Economic Forum (2020), the financial sector is one of the most targeted industries for cyberattacks, emphasizing the need for robust security measures. Cybersecurity threats include phishing, ransomware, data breaches, and account takeover attacks, which can lead to significant financial losses and reputational damage for banks[14].

One of the primary applications of AI and ML in digital banking is fraud detection. Traditional rule-based systems are often inadequate for identifying new and evolving threats. ML models, such as decision trees, neural networks, and ensemble methods, can learn from historical transaction data to detect fraudulent activities with higher accuracy. Research highlights the effectiveness of using supervised learning models for credit card fraud detection, achieving higher accuracy rates compared to traditional methods[16].

AI-driven behavioral analytics tools monitor user behavior to establish baseline patterns. Any deviation from these patterns can trigger alerts for potential fraud or account compromise. For example, if a user who typically logs in from one geographic location suddenly accesses their account from a different country, the system can flag this as suspicious. A study shows that integrating behavioral biometrics with machine learning models significantly improves the detection of account takeover attacks[15].

Future directions

The integration of AI and ML in cybersecurity within digital banking is poised for significant evolution, focusing on several key future directions that can enhance security and maintain customer trust. One crucial area is improving the explainability of AI models. As AI systems increasingly influence decision-making processes in cybersecurity, understanding how these models arrive at their conclusions is essential. This can foster trust among stakeholders and ensure compliance with regulatory standards. Future research should prioritize the development of Explainable AI (XAI) techniques, including model-agnostic methods like LIME and SHAP, which clarify predictions and highlight the important features driving model decisions.

Another vital direction is enhancing data privacy measures. Given the sensitivity of the data handled by banks, robust privacy protections are essential to safeguard customer information and comply with regulations such as GDPR. Research should explore the implementation of federated learning, allowing AI models to learn from decentralized data sources without transferring sensitive information. Additionally, employing differential privacy techniques can introduce noise to datasets, ensuring individual data points remain secure while still allowing for meaningful analysis. Promoting privacy-by-design frameworks in AI development will also help integrate privacy considerations throughout the entire lifecycle of AI systems.

Establishing robust frameworks for AI governance is equally important as AI systems become more prevalent in cybersecurity. Creating comprehensive governance frameworks that address ethical considerations in AI usage—such as fairness, accountability, and transparency—will ensure responsible application. Future research should focus on developing risk assessment models to evaluate potential biases and decision-making transparency, as well as compliance mechanisms for ongoing monitoring of AI systems against established regulations.

Collaboration among financial institutions, technology providers, and regulatory bodies is crucial in enhancing collective defense against cyber threats. Establishing public-

private partnerships can facilitate knowledge sharing and resource allocation, while forming industry consortiums can help develop common standards and protocols for AI and cybersecurity practices. Joint research initiatives involving academia, financial institutions, and technology providers can drive innovation and address shared challenges.

Lastly, continuous education and training will be essential as the technology landscape evolves. Developing training programs on AI and cybersecurity best practices can equip professionals across various roles with the necessary skills and knowledge. Public awareness campaigns can also promote understanding among customers regarding the role of AI in cybersecurity and empower them to take proactive measures against threats. By focusing on these key areas, the digital banking sector can strengthen its cybersecurity posture while ensuring compliance and maintaining customer trust in an increasingly digital world.

Conclusion:

In conclusion, the rapid expansion of digital banking has fundamentally transformed the financial landscape, delivering unmatched convenience and accessibility to consumers. Yet, this shift has concurrently amplified cybersecurity risks, with banks increasingly targeted by cybercriminals exploiting weaknesses in digital systems. This chapter underscores the vital importance of robust cybersecurity measures in protecting sensitive financial data, preventing fraud, and ensuring compliance with regulatory standards. By implementing strategies such as encryption, multi-factor authentication, biometrics, and comprehensive network security protocols, financial institutions can fortify their defenses against emerging threats like phishing, ransomware, and identity theft. Moreover, the integration of artificial intelligence (AI) and machine learning (ML) offers significant potential for improving threat detection and response capabilities in digital banking. As the digital banking landscape continues to evolve, adopting proactive cybersecurity strategies will be crucial in fostering trust, safeguarding assets, and ensuring the resilience of modern financial institutions against the constantly changing cyber threat environment.

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TRANSITION ELEMENTS AND ITS GENERAL CHARACTERISTICS

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Transition elements:

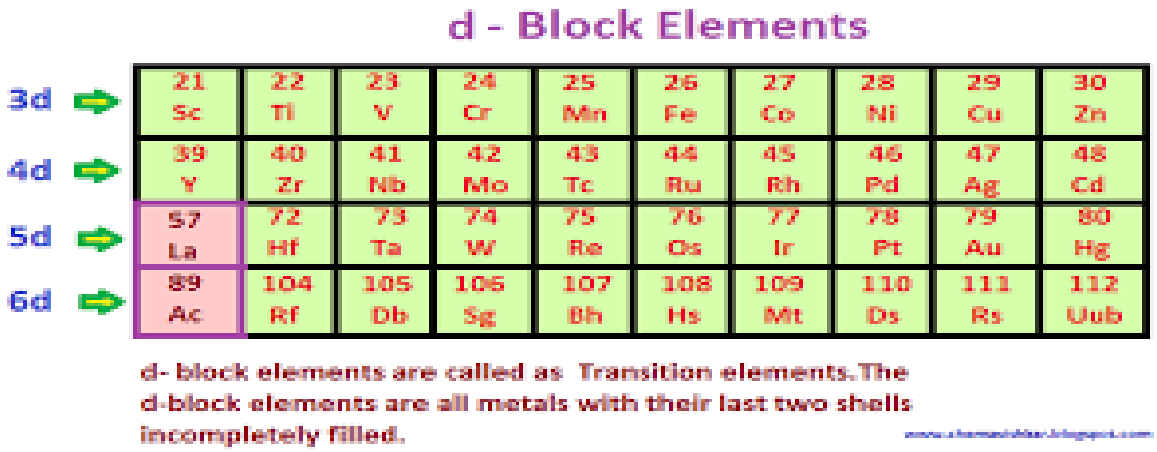
A transition element has incompletely filled d orbitals in its ground state or in any one of its oxidation states. The elements in which differentiating electron enter in (n-1) d orbitals of $(n-1)^{th}$ main shell are called transition elements or d-block elements . These elements are also known as bridge elements as they are lying between s and p block elements in a periodic table. Because the differentiating electron in these elements enters in d -orbital these elements are called as d-block elements. The d- block elements are called as transition elements because their properties are intermediate between the s-block and p-block elements. Elements from group-3 to group-12 belong to the d-block.

All d- block elements are not transition elements but all transition elements are d-block elements. All d- block elements are not transition elements because d-block elements like Zinc, Cadmium and Mercury have full d^{10} configuration in their ground state as well as in their common oxidation state which is not according to the definition of transition elements, but because of the resemblance of properties with d-block elements they are studied under the d-block. d-block elements are called transition elements as they show transition in the properties from the most electropositive s-block elements to the less electropositive p-block elements.

Position of transition elements in the periodic table:

Transition elements are found in the middle of the periodic table. Transition elements are placed in between the s and p block elements in the periodic table. As we move from left to right (from s- block to the p- block) the properties of transition elements change from ionic to covalent.

Transition elements have 10 groups (3-12) and 4 periods. The 4^{th} period is incomplete.



There are four series of elements which constitute the d-block elements. Each series comprises ten elements as given below:

1. Elements of the First Transition series or 3d-Transition series: The elements from scandium (Sc, Z = 21) to Zinc (Zn, Z = 30) form the 3d-series.
2. Elements of the Second Transition series or 4d-Transition series: This series consists of the elements from yttrium (Y, Z = 39) to cadmium (Cd, Z = 48).
3. Elements of the Third Transition series or 5d-Transition series: The elements lanthanum (La, Z= 57) and hafnium (Hf, Z= 72) to mercury (Hg, Z = 80) constitute the 5d-Transition series.
4. Elements of the Fourth Transition series or 6d-Transition series: The elements actinium (Ac, Z = 89) and rutherfordium (Rf, Z = 104) to copernicum (Cn, Z = 112) are the members of this series. All these elements are radioactive and do not occur in nature. These have been artificially made in the laboratory.

Electronic configuration of transition elements:

Electronic configuration of an element is characterized as an arrangement of electrons in the orbital. The d-block elements have a valence shell electronic configuration of (n-1) d $^{1\text{-}10}$ns $^{0\text{-}2}$ where (n-1) stands for inner shell whose d-orbitals may have one to ten electrons and the s-orbitals of the outermost shell (n) may have no electron or one or two electrons. The filling of d-orbitals takes place after the s-orbital of next higher shell has already been filled.

The general valence electronic configuration of transition elements is [Inert gas](n-1)$d^{1-10}ns^{1-2}$, where n is the highest principal quantum number of an occupied orbital in that atom.

The four series of d-block elements have the general electronic configuration as shown below:

(i) 3d series: [Ar] $3d^{1-10}\,4s^{1-2}$

(ii) 4d series: [Kr] $4d^{1-10}\,5s^{0-2}$

(iii) 5d series: [Xe] $5d^{1-10}\,6s^{2}$

(iv) 6d series: [Rn] $6d^{1-10}\,7s^{2}$

Electronic configuration of 3d Series:

Element	Symbol	Atomic Number	Electronic Configuration
Scandium	Sc	21	$[Ar]3d^{1}\,4s^{2}$
Titanium	Ti	22	$[Ar]3d^{2}\,4s^{2}$
Vanadium	V	23	$[Ar]3d^{3}\,4s^{2}$
Chromium	Cr	24	$[Ar]3d^{5}\,4s^{1}$
Manganese	Mn	25	$[Ar]3d^{5}\,4s^{2}$
Iron	Fe	26	$[Ar]3d^{6}\,4s^{2}$
Cobalt	Co	27	$[Ar]3d^{7}\,4s^{2}$
Nickel	Ni	28	$[Ar]3d^{8}\,4s^{2}$
Copper	Cu	29	$[Ar]3d^{10}\,4s^{1}$
Zinc	Zn	30	$[Ar]3d^{10}\,4s^{2}$

Cr (Z= 24): $3d^4\ 4s^2$ (expected but unstable) $3d^5\ 4s^1$ (actual, more stable).

Cu (Z=29): $3d^9\ 4s^2$ (expected but unstable) $3d^{10}4s^1$ (actual, more stable).

The electronic configuration of Chromium is $[Ar]3d^5 4s^1$ instead of $[Ar]3d^4 4s^2$. The electronic configuration of Copper is [Ar] $3d^{10}4s^1$ instead of [Ar] $3d^9 4s^2$. It is due to the additional stability gained by the atom when d-orbital is half filled in chromium or completely filled in copper. One electron is shifted from the lower level (4s) to the higher level (3d) in order to gain extra stability. As is evident, there is exchange of electrons from 4s to 3d subshell thereby increasing the stability of the valence shell configuration in Cr and Cu atoms. Thus, among 3d series elements, only Cr and Cu exhibit irregular/anomalous electronic configurations. Similarly, in 4d series, molybdenum has $4d^5 5s^1$ and silver has $4d^{10}5s^1$.

In higher elements, the energy difference between (n-1) d and ns orbitals become smaller and hence electron can jump from one orbital to other. Thus, there is irregularity in electronic configuration.

General characteristics (3d, 4d and 5d Series)

(i)Atomic radii and ionic radii

The transition elements are highly denser than the s- block elements. Their densities gradually decrease from scandium to copper because of an irregular decrease in metallic radii and a relative increase in atomic mass. The atomic radii generally decrease, with a few exceptions, on moving from left to right in each series of the transition elements due to increased nuclear charge at each step and constant value of the azimuthal quantum number (i.e.) receiving the last electron. The d-block elements have low atomic volumes as compared to those of the neighboring s- and p-block elements. This is due to the fact that in these elements (n-1) d-subshells are being filled and the increased nuclear charge pulls the electron cloud inwards.

As the atomic number increases the atomic radii actually decreases across a row in the periodic table due to the addition of extra electron to the same main energy level there is an increase in the effective nuclear charge. Within each group (vertical column), the atomic radius tends to increase with the atomic number.

Due to the screening effect, the size of atom does not alter much from chromium to copper and hence the atomic radii from chromium to copper are very close to each other. The successive addition of d-electrons screens outer electrons (4s electrons) from the inward pull by the nucleus.

Ionic Radii:

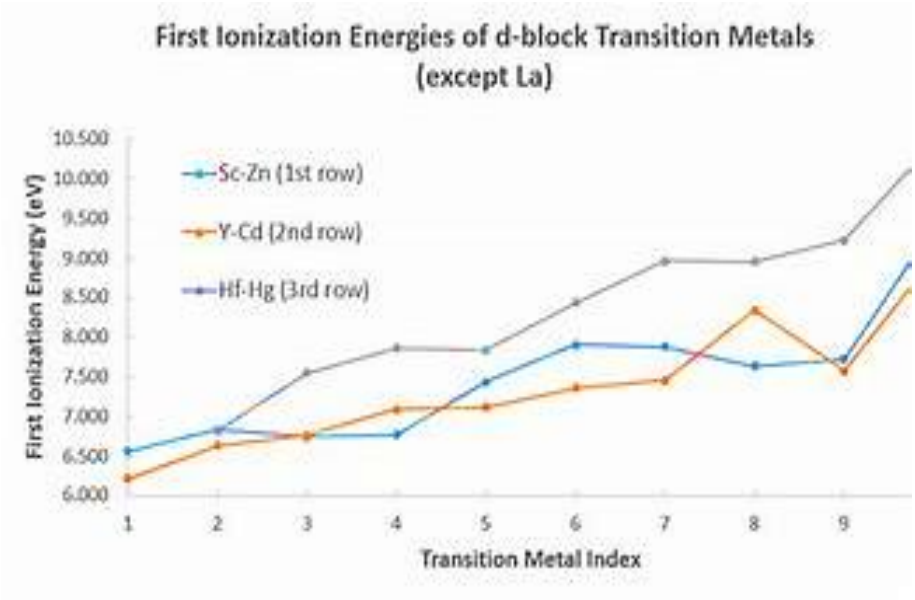
The radii of transition element cations are smaller than the radii of the corresponding metal atoms. For a given cation with charge M^{n+}, a small decrease in size is noticed in any given period. As the charge on the ion increases, the size of the cation decreases. The atomic radii and ionic radii of the 4d and 5d series are identical.

(ii)Ionization Energy (IE):

The minimum energy required to remove an electron from the ground state of atom (molecule) in the gas phase is its ionization energy. In simplest terms, the greater a metal's ionization energy, the harder it is to pull an electron from it.

The ionization potential of transition elements lies between s and p -block elements**.** They are less electropositive than the s-block elements. Henceforth, they do not frame ionic

compounds but form covalent compounds. They possess high ionization energy because of their small size. As the number of protons increase within a period (or row) of the periodic table, the first ionization energies of the transition-metal elements are relatively steady, while that for the main-group elements increases. The differing periodic trends in the effective nuclear charge are due to a greater increase in shielding in the transition-metal elements than in the main-group elements. Transition metals have smaller atomic radii and higher nuclear charge as compared to the alkali metals. The ionization energy increases due to the increase in the nuclear charge with atomic number at the beginning of the series. Second IE is always higher than first IE and it increases regularly.



Chromium and copper have high values of second IE than their neighbors because they have stable electronic configuration. After the formation of cation (M^+) remaining electrons are more tightly bound to nucleus. Removal of electrons from the ions Cr^+ and Cu^+ is difficult as they have $3d^5$ and $3d^{10}$ configuration, respectively. Hence removal of second electron requires more energy.

(iii)Variable oxidation states:

The first transition series elements generally show variable (many) oxidation states in their compounds / ionic forms. The cause of showing different oxidation states is that these elements have several 3d electrons which are quite close to 4s – electrons in energy. The minimum oxidation state shown by all the elements of this series is +2 except Cr and Cu which show +1 oxidation state as well. Higher oxidation states are due to the loss of one or more (n-1) d electrons in addition to ns electrons. The energy difference between ns

electrons and (n-1) d orbitals is small. Therefore, in addition to ns electrons, (n-1) d electrons can also be removed.

The number of oxidation states increases from Sc to Mn and then decreases till Zn which shows the +2-oxidation state only. As a result, among these elements, Cr and Mn show the maximum number of oxidation states from +1 to +6 and +2 to +7, respectively. From Sc to Mn, the highest oxidation state shown by any element is equal to the group number but the latter elements do not follow this trend. It is because the number of unpaired d electrons increases and after manganese pairing of d electrons starts.

It has been observed that the lower (+2, +3, etc.) oxidation states generally dominate the chemistry of the first transition series. For an element the relative stability of various oxidation states can be explained on the basis of the stability of d^0, d^5 and d^{10} configurations, e.g., Ti^{4+} ion ($3d^0\ 4s^0$) is more stable than Ti^{3+} ($3d^1\ 4s^0$) because of the presence of $3d^0$ subshell. Similarly, Mn^{2+} ($3d^5\ 4d^0$) ion is more stable than Mn^{3+} ($3d^4\ 4s^0$) ion since Mn^{2+} ion has $3d^5$ subshell.

The highest possible oxidation state, corresponding to the formal loss of all valence electrons, becomes increasingly less stable as we go from group 3 to group 8, and it is never observed in later groups. In the transition metals, the stability of higher oxidation states increases down a column.

Variable oxidation states of 3d series elements:

Element	Valence E.C	Oxidation States
Sc	$3d^1\ 4s^2$	+2, +3
Ti	$3d^2\ 4s^2$	+2, +3, +4
V	$3d^3\ 4s^2$	+2, +3, +4, +5
Cr	$3d^5\ 4s^1$	+1, +2, +3, +4, +5, +6
Mn	$3d^5\ 4s^2$	+2, +3, +4, +5, +6, +7
Fe	$3d^6\ 4s^2$	+2, +3, +4, +6
Co	$3d^7\ 4s^2$	+2, +3, +4
Ni	$3d^8\ 4s^2$	+2, +3
Cu	$3d^{10}\ 4s^1$	+1, +2
Zn	$3d^{10}\ 4s^2$	+2

(iv)Spectral properties:

When atoms or molecules absorb light at the proper frequency, their electrons are excited to higher-energy orbitals. For many main group atoms and molecules, the absorbed photons are in the ultraviolet range of the electromagnetic spectrum, which cannot be detected by the human eye.

The human eye perceives a mixture of all the colors, in the proportions present in sunlight, as white light. Complementary colors, those located across from each other on a color wheel, are also used in color vision. When a color is missing from white light, the eye sees its complement.

Transition metal complex ions and compounds are usually coloured when metal ion contain partially filled d-orbitals. When light consisting of many different colors falls on the coloured complex ion or compound, some portion of light is absorbed and remaining part is transmitted or reflected. Colour of absorbed light and colour of transmitted light are different from each other. These colours are called complementary colours. The colour of a given compound is the colour of the transmitted light.

Examples:

Hydrated copper (II) ion absorb yellow light and transmit blue light.
Hydrated titanium (III) ion absorb green light and transmit purple light.
Anhydrous cobalt (II) ion absorb red light and transmit blue-green light.
Hydrated cobalt (II) ion absorb blue-green light and transmit red light.

(v)Redox potential:

Redox potential is a measure of the propensity of a chemical or biological species to either acquire or lose electrons through ionization. In general, the ions of very late transition metals-- those towards the right-hand end of the transition metal block, such as copper, silver and gold have high reduction potentials. In other words, their ions are easily reduced. Standard electrode potential (SEP) of transition element is generally higher than that of standard hydrogen.

The irregularity in the variation of electrode potentials is due to the irregular variation of the ionisation enthalpies and also the hydration energies of the divalent ions of these elements. All those elements with negative reduction potentials act as strong reducing agents and liberate hydrogen from dilute acids. Copper does not liberate hydrogen from dilute acids because of its positive electrode potential. The values of the reduction potentials for Mn, Zn &Ni are more negative than expected. The electrode potential values of manganese and zinc can be explained on the basis of the stability of the half-filled d sub-shell in Mn^{+2}, and the completely filled d^{10} configuration in Zn^{+2}.

Standard electrode potentials for 3d-elements:

Element	E^0 (SRP) in volts
Sc	-2.10
Ti	-1.60
V	-1.20
Cr	-0.74
Mn	-1.18
Fe	-0.44
Co	-0.28
Ni	-0.25
Cu	+0.34
Zn	-0.76

There is no regular trend in the E° values. The metals should act as good reducing agents. This is because of irregular variation in the sublimation and ionization energies across the series.

(vi)Colour:

Colour of 3d transition metal ions:

Ion	Outer E.C	No. Unpaired Electrons	Colour
Sc^{3+}	$3d^0$	0	Colourless
Ti^{3+}	$3d^1$	1	Purple
Ti^{4+}	$3d^0$	0	Colourless
V^{3+}	$3d^2$	2	Green
Cr^{3+}	$3d^3$	3	Violet
Mn^{2+}	$3d^5$	5	Light Pink
Mn^{3+}	$3d^4$	4	Violet
Fe^{2+}	$3d^6$	4	Green
Fe^{3+}	$3d^5$	5	Yellow
Co^{3+}	$3d^7$	3	Pink
Ni^{2+}	$3d^8$	2	Green
Cu^{2+}	$3d^9$	1	Blue
Zn^{2+}	$3d^{10}$	0	Colourless

Colour of the substance arises from the property to absorb light of certain wavelength in the region of visible light (400-750 nm). If unpaired electrons are present in the ion, then its compound is coloured. If paired electrons are present in the ion, then its compound is colourless.

Colour exhibited by transition metal ions is due to the presence of unpaired electrons in d-orbitals and is due to the d-d transitions of electrons, when invisible light is incident on the ion. Colour of a complex depends on the metal, its oxidation state and its ligands, e.g., $[Cu(H_2O)_4]^{2+}$ is pale blue while $[Cu(NH_3)_4]^{2+}$ is dark blue. $CuSO_4 \cdot 5H_2O$ is blue in colour and anhydrous $CuSO_4$ is colourless.

(vii)Magnetic properties:

Magnetic Moment 3d transition metal ions:

Ion	Outer E.C	n	Magnetic Moment (BM)	
			Calculated	Observed
Sc^{3+}	$3d^0$	0	0.00	0.00
Ti^{2+}	$3d^1$	1	1.73	1.75
Ti^{3+}	$3d^2$	2	2.84	2.76
V^{2+}	$3d^3$	3	3.87	3.86
Cr^{2+}	$3d^4$	4	4.90	4.80
Mn^{2+}	$3d^5$	5	5.92	5.96
Fe^{2+}	$3d^6$	4	4.90	5-5.5
Co^{2+}	$3d^7$	3	3.87	4.4-5.2
Ni^{2+}	$3d^8$	2	2.84	2.9-3.4
Cu^{2+}	$3d^9$	1	1.73	1.4-2.2
Zn^{2+}	$3d^{10}$	0	0.00	0.00

Metal complexes that have unpaired electrons are magnetic. Since the last electrons reside in the d orbitals, this magnetism must be due to having unpaired d electrons. Many compounds of transition elements show magnetic properties. Compounds attracted by the magnetic field are paramagnetic.

Paramagnetic nature is due to the presence of unpaired electrons in d-orbitals. Paramagnetic character increases with increase in the number of unpaired electrons and

highest for Mn (II) [among 3d-series]. Compounds repelled by the magnetic field are diamagnetic.

The magnetic moment (μ) is expressed in terms of Bohr- Magneton (BM).

It is given by $1BM=eh/4\pi mC$.

With the help of the number of unpaired electrons, the magnetic moment is calculated using the formula

$\mu=\{n(n+2)\}^{1/2}$,

where n=number of unpaired electrons

(viii)Catalytic activity:

Many transition metals and complexes are used as catalysts which influence the rate of chemical reaction. The rate of a chemical reaction increases by the decrease in activation energy of the reactants. This decrease is caused by the catalyst which probably alter the path of the reaction. Bonds are formed between reactant molecules and atoms on the surface of the catalyst (first row transition metals utilize 3d and 4s-electrons for bonding). This results in the formation of reaction intermediates which provides path of lower activation energy and therefore, increase the rate of the reaction.

$A + B + C \rightarrow [A{-}B{-}C] \rightarrow A - B + C$

Reactants Catalyst Intermediate Product Catalyst

These reaction intermediates decompose to form the product(s) and regenerate the original catalyst.

Transition metals show catalytic behavior mainly due to the following reasons:

- The presence of vacant d orbitals.
- They have the ability to exhibit variable valencies.
- They have a tendency to form complex compounds

Examples of Transition metals as catalysts:

- Iron in the Haber Process.
- Nickel in the hydrogenation of C=C bonds.
- Vanadium(V) oxide in the Contact Process.
- Iron ions in the reaction between persulphate ions and iodide ions.
- Cu/V is used in the large-scale production of Nylon-66

(ix)Complex formation:

Transition metal complexes or coordination complexes are molecules that contain groups arranged around a central metal ion. In a way, these are like "lego-molecules", easily assembled from smaller parts, and sometimes they are easily transformed into new

molecules by switching out old parts for new ones. Transition metal complexes offer two distinct advantages as DNA-binding agents.

The transition metals form complexes due to two factors:

i. Metal ion is very small in size and has high positive charge density. It can accept lone pair of electrons from molecules or ions called ligands.
ii. They have vacant orbitals and these orbitals have right type of energy to accept lone pair of electrons Hexaamminecobalt (III) chloride, $[Co(NH_3)_6]Cl_3$, is an example of a coordination complex.

(x)Interstitial compounds:

A number of interstitial compounds are formed by the transition metals. The d-block elements form interstitial compounds with small non-metal atoms such as H, C, N, B, Si, etc. due to the ability of metal lattice to accommodate these non– metal atoms between the metal atoms without distortion of structure. As vacant spaces of the transition metals are filled up by small atoms, these compounds are hard and rigid. One of the striking properties of these metals is the formation of non-stoichiometric compounds which often exhibit semi conductivity, fluorescence and behave as heterogeneous catalysts. This non-stoichiometry is due to the defects in the solids.

Example: Iron (II) Oxide, the actual analysis shows that the formula varies between$Fe_{0.84}O$ to $Fe_{0.94}O$.

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ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN RESEARCH

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Abstract:

The integration of Artificial Intelligence (AI) and Machine Learning (ML) in scientific research is revolutionizing the landscape of knowledge discovery and innovation across diverse fields. This chapter explores the fundamental principles, methodologies, and applications of AI and ML in research, highlighting their transformative impact on modern science. It provides an in-depth analysis of how these technologies enhance data processing, accelerate hypothesis generation, and enable predictive modeling, thus fostering efficiency and accuracy in scientific inquiry. Key to this transformation is the ability of AI and ML algorithms to analyze vast and complex datasets, often referred to as "big data," that would be insurmountable using traditional research techniques. By automating processes like data classification, pattern recognition, and anomaly detection, AI and ML empower researchers to focus on higher-level cognitive tasks such as formulating novel hypotheses and designing innovative experiments. This chapter delves into supervised and unsupervised learning, neural networks, reinforcement learning, and deep learning architectures, emphasizing their role in solving intricate scientific challenges. Special attention is given to the role of AI and ML in disciplines such as materials science, biomedical research, chemistry, and physics, where AI-driven models are instrumental in discovering new materials, predicting molecular interactions, and optimizing experimental outcomes. Additionally, the ethical considerations, limitations, and potential biases associated with AI-driven research are critically examined. The chapter concludes by discussing future trends and opportunities, suggesting that AI and ML will continue to evolve as essential tools in research, not only augmenting human capabilities but also

potentially redefining the scope of scientific discovery itself. Through examples and case studies, this chapter illustrates the profound impact that AI and ML technologies are having on reshaping the methodology and trajectory of scientific exploration.

The chapter explores the intersection of AI with materials science, where machine learning algorithms have become indispensable tools for discovering and optimizing new materials. One notable case study includes AI's role in the accelerated discovery of high-performance alloys used in aerospace and energy applications. By processing large datasets of material properties, ML models predict material behavior and optimize performance, reducing the time for new material development from years to mere months. Another example is AI's contribution to battery material design, where it has helped in predicting the electrochemical properties of new materials for next-generation batteries. In biomedicine and drug discovery, AI is revolutionizing how pharmaceutical companies identify potential drug candidates. By leveraging ML models to predict molecular interactions and protein folding patterns, AI has reduced the time and cost of drug development significantly. One notable success is AlphaFold; a deep learning system developed by DeepMind that accurately predicts 3D protein structures from amino acid sequences. AI has also been instrumental in personalized medicine, enabling the development of patient-specific treatment plans by analyzing genetic, environmental, and lifestyle data. Climate science and environmental research are also benefitting from AI advancements. Machine learning is used for climate modeling, helping researchers simulate complex climate systems with greater accuracy. AI has been applied in predicting extreme weather events, monitoring deforestation, and optimizing energy consumption. For example, AI-driven models have optimized the performance of renewable energy systems, predicting wind and solar energy outputs, thereby improving the integration of renewable resources into energy grids. In chemistry, AI enhances the ability to predict the outcomes of chemical reactions, accelerating the synthesis of new compounds and improving the efficiency of chemical processes. ML algorithms are particularly useful in catalyst design—they have helped researchers discover new catalysts that accelerate chemical reactions, such as in sustainable energy processes like hydrogen production. AI also enables predictive modeling for chemical synthesis pathways, allowing researchers to design new molecules with desired properties more efficiently. In physics and astronomy, AI's capabilities are changing the way scientists analyze and interpret large datasets. AI has been critical in gravitational wave detection, where ML models sift through vast amounts of

observational data to identify signals that would otherwise be missed. AI has also been used in the search for exoplanets, identifying potential candidates by analyzing light curves from stars. These applications illustrate how AI can accelerate discoveries by automating the processing of complex, high-volume data. The chapter also addresses critical ethical considerations associated with the use of AI in research. The challenges of bias in AI models and the need for interpretability in machine-driven decisions are highlighted. For example, in healthcare and drug development, biased data can lead to models that do not generalize well to diverse populations, leading to inequities in treatment. Case studies in bias mitigation and ethical AI practices provide insights into how researchers can build more fair and transparent AI models. The chapter concludes with a forward-looking perspective, emphasizing that AI and ML will continue to evolve as essential tools in scientific research. As AI models become more sophisticated and their integration with experimental data deepens, the scope of scientific discovery will expand beyond what is currently imaginable. Case studies across multiple fields illustrate how AI-driven technologies have already begun to reshape the research landscape, setting the stage for even more profound breakthroughs in the future.

Introduction:

Artificial Intelligence and Machine Learning are at the forefront of a technological revolution that is reshaping science and technology research. Their impact is profound and widespread, affecting disciplines as varied as biology, chemistry, physics, and engineering. AI and ML provide tools that allow researchers to solve complex problems, analyze massive datasets, and make predictions that were previously impossible due to the limitations of traditional approaches. Artificial intelligence and machine learning are revolutionizing the way scientists conduct research, from data analysis to hypothesis generation. These technologies have the potential to accelerate scientific discovery, improve research efficiency, and uncover new insights that may not be possible through traditional methods. This chapter explores the roles of AI and ML in scientific research, illustrating how these technologies are advancing knowledge and innovation.

Understanding artificial intelligence and machine learning

Artificial Intelligence refers to the simulation of human intelligence in machines that are programmed to think, learn, and solve problems autonomously. It encompasses a wide range of capabilities, from simple automation to sophisticated systems capable of cognitive tasks such as reasoning and decision-making. Machine Learning, a subset of AI, focuses on

algorithms and statistical models that allow computers to perform tasks without explicit programming. In ML, the machine is trained using data to identify patterns and make predictions. There are several types of ML, including:

Supervised learning

Supervised learning, a widely-used machine learning technique, is applied in many industries like finance, healthcare, marketing, and others. A type of machine learning involves training the algorithm with labeled data to predict or make decisions based on data inputs. In supervised learning, the algorithm is taught how to map input data to output data. The mapping is obtained from a labeled dataset containing pairs of input and output data. The algorithm aims to understand the connection between the input and output data in order to predict new, unseen data with accuracy. Algorithms like linear regression, decision trees, and neural networks are trained on labeled datasets to predict material properties or optimize compositions. Supervised learning accounts for a lot of research activity in machine learning and many supervised learning techniques have found application in the processing of multimedia content. The defining characteristic of supervised learning is the availability of annotated training data. The name invokes the idea of a 'supervisor' that instructs the learning system on the labels to associate with training examples. Typically these labels are class labels in classification problems. Supervised learning algorithms induce models from these training data and these models can be used to classify other unlabelled data (Cunningham *et al.,* 2008). Storing and using specific instances improves the performance of several supervised learning algorithms. These include algorithms that learn decision trees, classification rules, and distributed networks. However, no investigation has analyzed algorithms that use only specific instances to solve incremental learning tasks (Aha *et al.,* 1991).

Unsupervised learning

Unsupervised learning, a basic form of machine learning, is constantly developing. This method, concentrating on input vectors lacking corresponding target values, has made significant progress in grouping and interpreting information through similarities, patterns, and differences. Recent progress in sophisticated unsupervised learning algorithms has improved this capability, allowing for a deeper understanding of intricate datasets. By 2024, unsupervised learning algorithms have further enhanced their autonomy and efficiency in uncovering the hidden patterns within unlabeled data, despite their lack of dependency on input-output mappings. The emergence of advanced self-

supervised learning methods has further enhanced the independence from relying on labeled data, diminishing the need for 'a teacher'.

Moreover, advancements have been made in combining unsupervised learning with other areas of AI, like reinforcement learning, resulting in smarter and more flexible systems. These systems are highly effective at recognizing patterns and irregularities in data, leading to the development of creative applications in different industries. This article delves deeper into unsupervised learning, discussing the different types and their applications. Techniques such as clustering and dimensionality reduction help in identifying patterns and structures in unlabeled data, useful for categorizing materials and discovering novel material families. Unlike supervised learning techniques, unsupervised learning methods do not use the output data for given inputs (also called labeled data) to train themselves, but they are designed to recognize the desired patterns from the available set of information. Unsupervised learning is basically the process of classifying data points that have similar “properties” to find a pattern to detect anomaly or to facilitate further processing of the data.

Reinforcement learning

Reinforcement learning, like other topics ending in -in like machine learning, planning, and mountaineering, is both a problem, a set of solution methods that are effective for that problem, and the field that researches these problems and solutions. Reinforcement learning tasks entail figuring out the optimal actions to take in different situations in order to maximize a numerical reward signal. Essentially, they are closed-loop issues because the actions of the learning system impact its future inputs. Additionally, the student is not instructed on which steps to follow, as is common in various types of machine learning. Instead, the student must determine which steps result in the highest reward through trial and error. In the most captivating and demanding scenarios, actions can impact not just the immediate outcome but also the following situation and, consequently, all future rewards. These three qualities--being essential in a closed-loop manner, lacking direct instructions on actions to take, and involving consequences and rewards over extended periods--is the primary distinguishing factors in reinforcement learning problems. This approach involves training algorithms to make sequential decisions, ideal for optimizing processes such as material synthesis pathways.

Reinforcement learning differs from unsupervised learning, where the focus is on discovering patterns within unlabelled datasets, as referred to by machine learning

experts. The terms supervised learning and unsupervised learning seems to cover all machine learning approaches, but they don't. Even though some may view reinforcement learning as similar to unsupervised learning since it doesn't require examples of correct behavior, its goal is to maximize a reward signal rather than uncover hidden patterns. Although identifying patterns in an agent's interactions can be beneficial in reinforcement learning, it alone does not solve the issue faced by the reinforcement learning agent. Therefore, we view reinforcement learning as a third type of machine learning, in addition to supervised and unsupervised learning, possibly along with other paradigms. Advances in machine learning algorithms and increased computational efficiencies give engineers new capabilities and tools to apply to engineering design. Machine learning models can approximate complex functions and, therefore, can be useful for various tasks in the engineering design workflow (Nathan *et al.,* 2022).

Neural networks and deep learning

Neural Networks are models used in computing that imitate the intricate functions of the human brain. Neural networks are composed of interconnected neurons that analyze and learn from data, allowing for tasks like pattern recognition and decision-making in machine learning. The article delves deeper into neural networks, including their functionalities, structure, and additional information. Neural networks identify features in data without pre-programmed knowledge. Components of a network consist of neurons, connections, weights, biases, propagation functions, and a learning rule. Neurons receive inputs based on thresholds and activation functions. Connections include weights and biases that control the flow of information. The process of learning and adapting weights and biases takes place in three phases: input calculation, generating output, and continuously improving to enhance the network's effectiveness in various tasks. The game of Go has long been viewed as the most challenging of classic games for artificial intelligence owing to its enormous search space and the difficulty of evaluating board positions and moves (Silver, D., *et al.,* 2016).

Neural networks' capability to recognize patterns, solve complex puzzles, and adapt to evolving environments is crucial. Their ability to acquire knowledge from data has wide-ranging impacts, transforming fields such as natural language processing and autonomous vehicles, as well as streamlining decision-making and improving efficiency across various sectors. The progress of artificial intelligence heavily relies on neural networks, which play a key role in driving innovation and shaping the course of technology. Deep learning, a

subset of ML, employs neural networks with multiple layers (deep neural networks) to model complex relationships in data. Convolutional neural networks (CNNs) and recurrent neural networks (RNNs) are particularly effective for image and sequence data, respectively, enabling tasks such as microstructure analysis and time-series prediction in material science.

Deep learning algorithms are a subset of the machine learning algorithms, which aim at discovering multiple levels of distributed representations. Recently, numerous deep learning algorithms have been proposed to solve traditional artificial intelligence problems (Guo, Y., Liu, Y., Oerlemans, A., *et al.,* 2016). Deep learning is a branch of machine learning that utilizes deep neural networks, consisting of multiple layers, to mimic the intricate decision-making capabilities of the human brain. Most AI applications in our daily lives are fuelled by some kind of deep learning. The main distinction between deep learning and machine learning lies in the design of the neural network framework. "Shallow," conventional machine learning models utilize basic neural networks with just one or two computational layers. Deep learning models utilize three or more layers, but often incorporate hundreds or even thousands of layers in the training process.

Supervised learning models need organized, labeled data to produce precise results, whereas unsupervised learning can be utilized by deep learning models. Unsupervised deep learning enables models to extract necessary characteristics, features, and relationships from raw, unstructured data for accurate outputs. Furthermore, these models have the capability to assess and improve their results for enhanced accuracy. Deep learning in data science powers numerous applications and services that enhance automation by carrying out analytical and physical tasks without human involvement. This allows for a wide range of common items and services to function, including digital assistants, voice-controlled TV remotes and fraud detection for credit cards, self-driving vehicles and generative AI.

Artificial neural networks, also known as neural networks, aim to replicate the human brain by utilizing data inputs, weights, and bias, which function as silicon neurons. These components collaborate to precisely identify, categorize, and explain items in the information. Deep neural networks comprise numerous layers of linked nodes, with each layer enhancing and improving predictions or categorizations based on the preceding layer. Forward propagation is the term used to describe the process of computations moving through the network. The visible layers of a deep neural network are referred to as

the input and output layers. The data is received and processed by the deep learning model in the input layer, while the final prediction or classification is produced in the output layer. Another technique known as back propagation utilizes algorithms like gradient descent to compute errors in predictions and subsequently modifies the weights and biases of the function by iterating backwards through the layers to train the model. Combined, forward and backward propagation allow a neural network to predict outcomes and rectify mistakes. As time passes, the algorithm improves in accuracy. Extensive computing power is essential for deep learning. Highly efficient graphical processing units (GPUs) are perfect as they are capable of managing a vast quantity of calculations across numerous cores with ample memory at their disposal. Distributed cloud computing could also provide help. This amount of computing power is essential for training deep algorithms using deep learning. Nevertheless, overseeing numerous GPUs on site could place a significant strain on internal resources and prove to be quite expensive when it comes to expansion. When it comes to software needs, the majority of deep learning applications are developed using one of these three learning frameworks: JAX, PyTorch, or TensorFlow.

These technologies have evolved rapidly, leading to breakthroughs in fields such as image recognition (He, K., Zhang, X., Ren, S., & Sun, J., 2016), natural language processing and robotics.

AI and ML in biology and medicine

AI and ML have revolutionized the field of biology and medicine, particularly in areas such as genomics, drug discovery, and diagnostics. The integration of Artificial Intelligence and Machine Learning into biology and medicine is heralding a new era of scientific discovery and healthcare advancements. These technologies enable researchers and healthcare professionals to analyze vast datasets, make predictions, and automate processes that were once considered time-intensive or beyond human capability (Rajkomar, A., Dean, J., & Kohane, I., 2019). In particular, AI and ML are playing transformative roles in genomics, drug discovery, and medical diagnostics. This section aims to provide an in-depth exploration of how AI and ML are revolutionizing these critical fields. Outfitted with deep neural networks, mobile devices can potentially extend the reach of dermatologists outside of the clinic (Esteva, A., *et al.,* 2017). The use of artificial intelligence and the deep-learning subtype in particular, has been enabled by the use of labeled big data, along with markedly enhanced computing power and cloud storage, across all sectors. In medicine, this is beginning to have an impact at three levels: for

clinicians, predominantly via rapid, accurate image interpretation; for health systems, by improving workflow and the potential for reducing medical errors; and for patients, by enabling them to process their own data to promote health (Topol, E. J. (2019).

AI and ML in genomics

One of the most significant breakthroughs facilitated by AI is in genomics. The sheer volume of genetic data generated from high-throughput sequencing methods such as next-generation sequencing (NGS) requires powerful computational tools for analysis. AI and ML algorithms can process these large datasets, identifying patterns in genetic variations, predicting phenotypes and even pinpointing disease-causing mutations. For instance, AI was instrumental in the success of the Human Genome Project, and today, machine learning models are helping to analyze single-cell RNA sequencing data, which reveals gene expression at the cellular level. This is critical in understanding complex biological processes such as cancer progression, where tumors consist of genetically heterogeneous cell populations.

The field of genomics has witnessed tremendous advancements with the application of AI and ML, especially in the processing of large-scale genomic data. High-throughput sequencing technologies, such as next-generation sequencing (NGS), generate enormous amounts of data that require advanced computational tools for interpretation. One of the most profound applications is the identification of disease-causing genetic variants. AI algorithms, trained on large datasets of known genetic mutations, can identify patterns that indicate which variants are likely to be pathogenic. This has important implications for understanding diseases like cancer, where mutations in specific genes can lead to uncontrolled cell growth. AI-powered tools also play a significant role in personalized medicine. By analyzing an individual's genetic profile, AI can help predict responses to drugs and tailor treatment strategies accordingly. This personalized approach to treatment is exemplified in pharmacogenomics, where AI models predict how patients will metabolize certain medications based on their genetic makeup, leading to more effective and safer treatments. Moreover, single-cell RNA sequencing (scRNA-seq) data, which provides insights into gene expression at the cellular level, has been a key area where machine learning algorithms excel. By clustering cells based on gene expression profiles, AI can reveal previously unrecognized cellular subtypes, offering deeper insights into developmental biology and disease progression, such as in the case of tumor heterogeneity in cancer research.

AI and ML in drug discovery

Drug discovery has traditionally been a time-consuming and expensive process, with a high failure rate. AI and ML are transforming this field by accelerating the identification of potential drug candidates and optimizing drug design. By analyzing molecular data, AI systems can predict how different compounds will interact with biological targets, vastly improving the speed of screening processes. An example of this is AlphaFold, a deep learning model developed by DeepMind that can predict the three-dimensional structures of proteins from their amino acid sequences with remarkable accuracy. The prediction of protein structures is critical in understanding diseases and designing new drugs. In 2020, AlphaFold made headlines by achieving a level of precision comparable to experimental methods like X-ray crystallography, which was previously considered the gold standard in structural biology. Furthermore, companies like Insilico Medicine use AI to design drugs that target specific pathways involved in diseases like cancer and fibrosis. By employing generative models, Insilico Medicine can create novel molecules that have the desired properties to interact with these targets, which accelerates the process of bringing new drugs to clinical trials.

Drug discovery is one of the most challenging and resource-intensive aspects of biomedical research. Traditional methods often involve laborious trial-and-error processes. AI and ML are revolutionizing this space by significantly speeding up the identification of new drug candidates and optimizing the drug development pipeline. One notable breakthrough has been the development of AlphaFold, an AI model created by DeepMind. AlphaFold has made significant strides in predicting protein structures from amino acid sequences, a problem that had long stymied scientists (Jumper, J., *et al.,* 2021. Understanding the 3D structure of proteins is crucial for drug discovery, as it allows researchers to design drugs that specifically target disease-causing proteins. The accuracy with which AlphaFold predicts these structures is comparable to experimental techniques like X-ray crystallography, which are more time-consuming and costly. Furthermore, AI models are being used to screen millions of chemical compounds to identify potential drug candidates. Traditional screening methods are costly and time-intensive, but AI can narrow down the vast chemical space to the most promising compounds. For example, companies like Atom wise use deep learning models to predict how small molecules will interact with specific protein targets, dramatically speeding up the process of lead compound identification. Beyond the initial stages of drug discovery, machine learning also plays a

vital role in clinical trials. By analyzing patient data, AI can identify optimal trial designs, predict patient outcomes, and even recommend adjustments to dosages in real-time to improve safety and efficacy. This level of precision could significantly reduce the time and cost associated with bringing new therapies to market.

AI and ML in medical diagnostics and imaging

Medical imaging is another area where AI and ML have shown exceptional promise. Traditional diagnostic tools, such as X-rays, MRIs, and CT scans, generate vast amounts of data that can be time-consuming for radiologists to analyze. AI-powered systems can automate the analysis of these images, identifying patterns that are difficult for humans to detect and improving diagnostic accuracy. AI-driven platforms, such as Zebra Medical Vision and Arterys, have been developed to assist radiologists by detecting diseases like cancer, cardiovascular abnormalities, and neurological disorders. These systems use convolutional neural networks (CNNs), a type of deep learning algorithm particularly effective at processing image data. AI systems trained on large datasets of medical images have demonstrated performance levels on par with, and sometimes even exceeding, human experts. AI also plays a role in predictive diagnostics. Machine learning models can analyze patient data, including genetic information, electronic health records, and lifestyle factors, to predict the likelihood of developing diseases like diabetes, heart disease, or cancer. This allows for earlier intervention and personalized treatment plans, improving patient outcomes.

AI's ability to analyze vast amounts of data in a short time makes it an ideal tool for diagnostics, particularly in the field of medical imaging. Modern medical imaging techniques, such as CT scans, MRIs, and X-rays, produce an enormous volume of images that require careful analysis. AI algorithms, particularly those based on convolutional neural networks (CNNs), are now being trained to analyze these images with a high degree of accuracy. In radiology, AI systems can detect abnormalities such as tumors, fractures, or lesions with a precision comparable to, or even exceeding, that of human radiologists. Companies like Zebra Medical Vision and Aidoc have developed AI-powered systems that can identify signs of various diseases, including cancer and cardiovascular conditions, from medical images. These systems not only improve the speed and accuracy of diagnoses but also reduce the workload on healthcare professionals, allowing them to focus on more complex cases. AI and ML are also enabling early detection of diseases. For instance, AI algorithms trained on electronic health records (EHRs) and genomic data can predict the

likelihood of a patient developing chronic conditions such as diabetes, heart disease, or Alzheimer's. This allows for early interventions that can significantly improve patient outcomes. Moreover, in pathology, AI tools are being employed to analyze tissue samples for cancer diagnosis. Traditionally, this has been a labor-intensive process requiring expert pathologists to examine tissue slides under a microscope. Now, AI systems can analyze digitized slides, identifying subtle patterns and features that might escape the human eye, leading to faster and more accurate diagnoses.

Applications of AI in predictive healthcare

Predictive healthcare is another area where AI and ML have shown significant potential. By analyzing various data sources, including medical records, lifestyle data, and genetic information, AI systems can predict the onset of diseases and suggest preventive measures. For example, AI models can predict the likelihood of a patient developing cardiovascular diseases based on their medical history, blood pressure levels, and lifestyle habits. Early interventions, such as lifestyle changes or preventive medications, can then be recommended to reduce the risk of severe outcomes. Predictive analytics is also playing an increasingly important role in hospital management, helping healthcare institutions optimize patient care and resource allocation. AI can predict patient admissions, emergency room visits, and ICU occupancy, allowing hospitals to manage resources more efficiently.

AI and ML in telemedicine and remote monitoring

The rise of telemedicine has been greatly supported by AI and ML technologies, particularly in the context of remote patient monitoring. Wearable devices such as smart watches and fitness trackers continuously collect data on vital signs like heart rate, blood pressure, and oxygen levels. Machine learning algorithms analyze this data in real-time, alerting both patients and healthcare providers to any irregularities or potential health issues. For example, patients with chronic conditions like diabetes or hypertension can use AI-powered platforms to monitor their health at home, reducing the need for frequent hospital visits. These systems can detect abnormal readings and prompt the patient to take specific actions, such as adjusting medication or seeking medical attention. This continuous monitoring enables more personalized healthcare and can prevent complications by catching issues early. AI is also transforming virtual consultations. Natural language processing (NLP) algorithms enable AI systems to interact with patients, gathering information about their symptoms and medical history before a virtual appointment. This

helps doctors make more informed decisions during consultations and improves the overall efficiency of the telemedicine process.

Challenges and ethical considerations

While the application of AI and ML in biology and medicine offers immense potential, there are several challenges and ethical considerations that must be addressed. One major challenge is the interpretability of AI models. Many AI systems, particularly those based on deep learning; function as "black boxes," meaning that it is difficult to understand how they arrive at their predictions. This lack of transparency can be problematic, especially in medical settings where the reasons behind a decision (such as a diagnosis) need to be clearly understood by healthcare providers. Data privacy is another critical concern. The use of patient data to train AI models raises questions about how this sensitive information is stored, shared, and protected. Ensuring that patient data is handled responsibly and in compliance with regulations like the General Data Protection Regulation (GDPR) which is paramount to maintaining trust in AI-driven healthcare solutions. Finally, there is the issue of bias in AI models. If an AI system is trained on data that is not representative of the broader population, it may produce biased outcomes that disproportionately affect certain groups. This has serious implications in healthcare, where biased AI systems could lead to disparities in treatment or diagnosis.

AI and ML are transforming the fields of biology and medicine, offering unprecedented opportunities for improving diagnostics, drug discovery, and personalized medicine. These technologies are enabling researchers and healthcare professionals to address complex challenges, make more accurate predictions, and develop innovative solutions for pressing medical issues. However, as AI continues to play a larger role in these fields, it is crucial to address the challenges and ethical concerns that accompany its use. By doing so, AI and ML can fully realize their potential to improve patient outcomes and advance biomedical research.

AI and ML in physics and chemistry

In the physical sciences, AI and ML are playing an increasingly important role in solving complex problems, especially in areas where traditional analytical techniques fall short. Artificial Intelligence and Machine Learning are significantly impacting the fields of physics and chemistry, offering new ways to solve complex problems, simulate systems, and predict the properties of materials and molecules. These technologies have enhanced the precision and speed of research in areas such as quantum physics, materials discovery,

and chemical reactions. This section explores the application of AI and ML in both fields, emphasizing their transformative potential in theory, experimentation, and industrial application.

AI and ML in quantum physics

Quantum physics deals with the behavior of matter and energy at atomic and subatomic scales, where traditional computational methods often fail due to the enormous complexity of quantum systems. AI and ML provide powerful tools to tackle these challenges, especially in quantum mechanics and quantum computing. In quantum physics, AI and ML are used to model complex quantum systems. These systems are notoriously difficult to study due to the exponential growth of variables as system size increases. By leveraging AI, researchers can simulate quantum interactions more efficiently, providing insights into the behavior of particles at the quantum level. For example, quantum machine learning (QML) combines quantum computing with ML algorithms to solve problems in material science and cryptography that classical computers struggle with. Google AI Quantum and IBM Q are leading projects in this area, developing quantum algorithms that promise to accelerate research in fields such as materials discovery and quantum chemistry.

Quantum simulations

In quantum physics, simulating quantum systems—particularly large, multi-particle systems is notoriously difficult due to the exponential growth of variables. Classical computers struggle to handle the vast array of possible quantum states, but AI and ML have provided new approaches to simulate these systems efficiently. Machine learning algorithms, particularly reinforcement learning and neural networks, are being employed to model the behavior of particles and predict outcomes in quantum systems. For example, variational quantum eigensolvers (VQEs), which use quantum circuits in combination with ML techniques, allow researchers to approximate the ground state of molecules, which is essential in understanding chemical reactions and material properties. AI's ability to optimize quantum circuit parameters drastically reduces the computational cost of solving these quantum problems. Google's AI Quantum and IBM's Quantum Experience platforms are advancing the integration of quantum computing with machine learning algorithms. These systems are employed to simulate molecular structures, perform quantum chemistry calculations, and solve optimization problems that are intractable for classical computers.

Quantum Machine Learning (QML)

Quantum Machine Learning (QML) combines quantum computing with machine learning to enhance both fields. QML promises faster processing times for specific ML tasks like optimization, pattern recognition, and data analysis, which are essential in complex quantum systems. Quantum computers can, in principle, outperform classical computers in training certain ML models, like quantum support vector machines (QSVM) and quantum neural networks (QNNs). These models hold the potential to accelerate research in areas such as cryptography, material science, and pharmaceuticals by solving optimization problems that classical ML models would struggle with.

AI and ML in materials science

The discovery of new materials with desirable properties is central to advancing technology in sectors such as energy, electronics, and manufacturing. AI and ML have accelerated this process by enabling the design, prediction, and discovery of new materials more efficiently than traditional trial-and-error methods. AI and ML have also made significant strides in chemistry and materials science, particularly in the discovery of new materials with specific properties. Traditional methods of materials discovery rely on trial-and-error experimentation, which is time-consuming and resource-intensive. Machine learning models can accelerate this process by predicting the properties of materials based on their chemical composition. An example of AI's impact in this area is the discovery of new catalysts for chemical reactions. Catalysts are substances that speed up chemical reactions without being consumed in the process. Discovering new catalysts can revolutionize industrial processes, making them more efficient and environmentally friendly. ML models trained on databases of known catalysts can predict the properties of new materials, guiding experimental chemists toward more promising candidates for synthesis. AI has also been used to predict molecular stability, reactivity and other key chemical properties. For instance, Schrödinger is a company that uses AI-driven simulations to predict how molecules will behave in different environments, allowing for more accurate predictions in drug design and material science.

Predicting material properties

Materials science involves exploring vast combinations of elements to discover materials with specific characteristics, such as high conductivity, durability, or flexibility. AI and ML are now used to predict the properties of materials before they are synthesized, reducing the need for expensive and time-consuming experiments. ML models are trained

on large datasets of known materials and their properties to predict how new combinations of elements will behave under various conditions. For example, deep learning algorithms have been used to predict the thermal conductivity, elasticity, and electrical properties of new materials based on their atomic structure. This has dramatically accelerated the development of materials for applications in electronics, aerospace, and energy storage. A notable success in this area is the development of new high-performance alloys using ML. Companies like Citrine Informatics applies ML to analyze massive datasets on materials, helping industries discover new materials for use in clean energy technologies and other applications. Similarly, ML models are helping researchers design new photovoltaic materials for more efficient solar cells, contributing to advancements in renewable energy.

Materials discovery

AI and ML are also being used to discover new materials that would be difficult to identify through traditional methods. ML models can explore vast chemical and structural spaces, suggesting new material candidates for synthesis. In materials discovery, AI tools can scan databases and publications for relevant data, learning from both successes and failures in previous experiments. For example, AI-driven materials discovery has led to the identification of new catalysts for chemical reactions, which are critical in industrial processes like the production of fuels and chemicals. By analyzing large databases of catalytic reactions, ML algorithms can predict which combinations of materials will act as effective catalysts, thereby speeding up the development of more efficient and sustainable industrial processes. The Materials Genome Initiative, launched by the U.S. government, aims to leverage AI to accelerate the discovery of advanced materials. AI models trained on the vast dataset generated by the initiative can identify patterns and relationships between material properties, guiding experimentalists toward promising new materials for applications ranging from energy storage to advanced electronics.

AI and ML in chemical reactions

Chemical reactions are the foundation of chemistry, and understanding these reactions at a fundamental level is essential for developing new chemicals, pharmaceuticals, and industrial processes. AI and ML are revolutionizing this field by enabling the accurate prediction of chemical reactions and improving the efficiency of synthetic chemistry.

Predicting reaction outcomes

One of the key challenges in chemistry is predicting the outcome of a chemical reaction, including the yield, selectivity, and by-products. AI and ML models, particularly graph neural networks (GNNs) are being used to predict these outcomes by analyzing the structures of reactants and the conditions under which the reactions occur. By training on large datasets of chemical reactions, ML models can predict how new combinations of reactants will behave, reducing the need for trial-and-error experimentation. For example, IBM's RXN for Chemistry platform uses deep learning algorithms to predict the outcomes of chemical reactions, enabling chemists to design more efficient synthetic pathways. This has wide-ranging implications for the development of new pharmaceuticals, materials, and chemicals. AI-driven platforms like ChemProp and ASAP are also being employed to predict reaction yields and optimize reaction conditions, helping chemists maximize efficiency and reduce waste in chemical synthesis.

Automating chemical synthesis

AI and ML are also enabling the automation of chemical synthesis, which is critical in fields such as drug development and materials chemistry. Automated systems powered by AI can design and execute complex synthetic pathways, reducing the time and cost associated with developing new chemicals. For instance, autonomous laboratories equipped with AI-driven robots can perform thousands of chemical reactions, analyze the results, and adjust the experimental parameters in real-time to optimize the synthesis process. These systems can rapidly iterate through different reaction conditions, significantly accelerating the discovery of new compounds. DeepChem is one such platform that leverages deep learning to aid in the design and synthesis of new chemical compounds. Autonomous systems like MIT's automated molecular synthesis system use machine learning algorithms to determine the optimal route for synthesizing complex molecules. These systems have the potential to revolutionize fields like drug discovery, where the ability to rapidly synthesize and test new compounds is crucial.

AI and ML in theoretical chemistry

In theoretical chemistry, AI and ML have become indispensable for calculating the properties of molecules and predicting chemical behavior. One of the most promising applications of AI in this field is the use of ML models to approximate the solutions to the Schrödinger equation, which describes the quantum mechanical behavior of molecules. Traditional methods for solving the Schrödinger equation are computationally expensive

and impractical for large systems. However, AI algorithms, particularly neural networks and deep learning models, can approximate the solution to this equation more efficiently. For example, DeepMind's Deep Potential model has been used to calculate the energy landscapes of molecules, providing insights into their stability and reactivity. Moreover, AI-driven approaches are being used to calculate reaction mechanisms, predict molecular dynamics, and model the behavior of chemical systems in complex environments. These advancements are providing deeper insights into the fundamental principles governing chemical reactions and molecular behavior.

AI and ML in spectroscopy and analytical chemistry

AI and ML have significantly impacted spectroscopy and analytical chemistry, where they are used to analyze and interpret complex spectra. Spectroscopic techniques such as infrared (IR) spectroscopy, nuclear magnetic resonance (NMR), and mass spectrometry generate large datasets that require sophisticated tools for interpretation. AI algorithms, particularly those based on pattern recognition, can analyze these spectra to identify chemical compounds and predict molecular structures with high accuracy. In analytical chemistry, AI-powered systems are used to process large amounts of experimental data, helping chemists to quickly identify key trends and patterns. This enables faster decision-making and more efficient experimentation.

Challenges and ethical considerations

While AI and ML offer significant advantages in physics and chemistry, there are also challenges and ethical considerations that must be addressed. One of the key challenges is the interpretability of AI models. In many cases, AI algorithms, particularly deep learning models, function as "black boxes," meaning it is difficult to understand how they arrive at their predictions. This lack of transparency can be problematic, particularly in fields like drug discovery, where the reasoning behind decisions is critical. Another challenge is the quality of data. AI models rely on large datasets for training and the accuracy of these models depends on the quality of the data they are trained on. In fields like chemistry, where experimental data can be noisy or incomplete, ensuring the reliability of AI models is a key concern. Ethical considerations, particularly in the context of data privacy and bias are also relevant. Ensuring that AI models are fair, transparent, and reliable is essential for building trust in these technologies.

AI and ML are revolutionizing the fields of physics and chemistry by providing new tools for simulation, prediction, and discovery. In quantum physics, these technologies are

enabling the simulation of complex systems and the development of quantum machine learning algorithms. In chemistry, AI is accelerating the discovery of new materials, optimizing chemical reactions, and enabling the automation of synthetic processes. As AI and ML continue to evolve, they will play an increasingly important role in advancing scientific discovery and industrial applications in these fields.

AI and ML in engineering and robotics

Artificial Intelligence and Machine Learning are fundamentally transforming engineering and robotics, creating new possibilities for automation, optimization, and intelligent systems. The integration of AI and ML into these fields has led to more efficient processes, smarter machines, and the development of autonomous systems that can perform complex tasks with minimal human intervention. This chapter explores the applications of AI and ML in various engineering disciplines and robotics, highlighting how these technologies are driving innovation and changing the landscape of modern industry.

AI and ML in mechanical engineering

Mechanical engineering is a broad field that encompasses the design, analysis, and manufacturing of mechanical systems. AI and ML are being used to optimize design processes, enhance predictive maintenance, and improve manufacturing efficiency.

Design optimization and simulation

Traditionally, mechanical design relied on human expertise and iterative processes to optimize structures and systems. With the introduction of AI and ML, engineers now have tools that can automate the design process, allowing for faster and more efficient creation of components. Generative design is one such approach, where AI algorithms generate design alternatives based on predefined constraints and performance requirements. These algorithms can produce highly optimized designs that may not be intuitive to human engineers but meet performance criteria better than traditional designs. For instance, companies like Autodesk use AI to create optimized designs for lightweight structures in aerospace and automotive engineering, reducing material use while maintaining structural integrity. These algorithms can simulate thousands of design iterations, helping engineers choose the most efficient design faster than manual methods. AI and ML are also revolutionizing finite element analysis (FEA), a computational tool used to simulate how physical structures behave under different conditions. ML models can quickly predict the behavior of complex structures under stress, heat, or other forces, reducing the need for computationally expensive simulations.

Predictive maintenance

In mechanical engineering, AI-driven predictive maintenance systems are crucial for minimizing downtime and extending the lifespan of equipment. Predictive maintenance uses machine learning algorithms to analyze data from sensors placed on machinery to predict when failures are likely to occur. By analyzing vibration, temperature, and other operational data, these systems can forecast equipment breakdowns before they happen, allowing maintenance teams to address issues proactively. For example, companies like Siemens and GE have developed AI-based predictive maintenance solutions for industrial machines, turbines, and power plants. By leveraging historical data and real-time monitoring, these systems can predict machine failures and suggest maintenance schedules that minimize disruptions in production lines, improving efficiency and reducing costs.

AI and ML in civil engineering

In civil engineering, AI and ML are playing an increasingly important role in infrastructure design, construction management, and urban planning. These technologies are helping to build smarter cities and more resilient infrastructure by optimizing designs and improving decision-making processes.

Structural health monitoring

AI-based systems are being used to monitor the health of critical infrastructure, such as bridges, buildings, and dams. By analyzing data from sensors embedded in these structures, machine learning algorithms can detect early signs of stress, corrosion, or damage. This enables engineers to perform maintenance or repairs before issues become severe, reducing the risk of catastrophic failures. For example, AI-based monitoring systems have been deployed in long-span bridges like the Golden Gate Bridge to analyze stress data in real-time. ML algorithms process this data to detect any abnormalities in the bridge's structure, helping engineers maintain the safety and integrity of the infrastructure.

Smart city development

AI and ML are central to the development of smart cities where infrastructure and urban planning are optimized for sustainability, efficiency and livability. In smart cities, AI algorithms analyze data from sensors and Internet of Things (IoT) devices to manage resources like water, energy, and traffic flow. For example, AI can optimize traffic light patterns based on real-time traffic conditions, reducing congestion and improving fuel efficiency. In urban planning, AI-based systems are used to model city growth, predict infrastructure needs, and simulate the impact of new developments on transportation and

public services. Machine learning algorithms can analyze data from social media, satellite imagery, and economic indicators to provide insights into how cities should evolve to meet the needs of their populations.

AI and ML in electrical and electronic engineering

In electrical and electronic engineering, AI and ML are used in the design and optimization of electrical systems, power grids, and electronic devices. These technologies enable smarter energy management and the development of more efficient, autonomous systems.

Smart grid management

The power grid is becoming increasingly complex with the integration of renewable energy sources like solar and wind. AI and ML are essential for managing this complexity, ensuring a stable supply of electricity while minimizing costs and environmental impact. Smart grids use AI algorithms to predict electricity demand, optimize energy distribution, and integrate renewable energy sources into the grid. AI models analyze real-time data from energy producers, consumers and weather forecasts to balance electricity generation and consumption. For instance, machine learning algorithms can predict when wind or solar energy production will be high, allowing the grid to store excess energy or reduce the output of traditional power plants. This reduces reliance on fossil fuels and helps maintain grid stability.

Electronic Design Automation (EDA)

In the design of electronic devices, AI and ML are being used in Electronic Design Automation (EDA) tools to optimize circuits and microchips. These tools help engineers design complex electronic systems, such as integrated circuits (ICs) and printed circuit boards (PCBs), more efficiently. ML algorithms can predict how different design choices will affect performance, power consumption, and manufacturing costs, allowing for faster iterations in the design process. Companies like Synopsys and Cadence Design Systems are incorporating AI into their EDA tools, enabling engineers to design next-generation microchips used in smart phones, computers, and autonomous vehicles.

AI and ML in robotics

The field of robotics is perhaps the most visible example of AI and ML's impact on engineering. AI-powered robots are capable of performing complex tasks autonomously, from manufacturing and logistics to healthcare and exploration. Machine learning

algorithms enable robots to perceive their environment, make decisions, and learn from experience.

Autonomous robotics

Autonomous robots are designed to operate without human intervention, relying on AI and ML to navigate their surroundings, make decisions, and perform tasks. For example, self-driving cars, powered by AI-based perception and control systems, can interpret data from cameras, lidar and radar to navigate roads and avoid obstacles. Companies like Waymo and Tesla have developed advanced AI systems for autonomous driving, pushing the boundaries of what robots can achieve in the real world. Similarly, autonomous robots are being used in industrial settings, such as Amazon's robotic warehouses, where AI-powered robots navigate complex environments, pick items, and transport them efficiently. These robots use reinforcement learning algorithms to optimize their behavior, learning from their environment to improve task performance over time.

AI and ML are integral to the development of autonomous systems, such as self-driving cars, drones, and industrial robots. These systems rely on AI to navigate their environment, make decisions in real-time, and adapt to new situations. Reinforcement learning algorithms, in particular, are widely used to train robots to perform tasks autonomously by rewarding actions that lead to desired outcomes and penalizing those that do not. Autonomous robots are increasingly being used in industrial settings to perform tasks such as assembling products, monitoring infrastructure, and even conducting repairs. For instance, in the aerospace industry, autonomous drones equipped with AI systems can inspect aircraft, identifying defects or damage that would be difficult for human inspectors to detect. This improves safety and reduces downtime in the maintenance process.

Robotic manipulation and human-robot interaction

One of the key challenges in robotics is enabling robots to interact with objects and humans in dynamic, unstructured environments. Machine learning plays a crucial role in robotic manipulation, where robots are trained to pick up, move, and manipulate objects with precision. AI-based reinforcement learning algorithms allow robots to learn how to handle objects by trial and error, improving their dexterity and adaptability. For example, robots used in surgical applications, such as the da Vinci Surgical System are increasingly being augmented with AI capabilities that assist surgeons in performing complex procedures with high precision. Human-robot interaction (HRI) is another area where AI

and ML are making significant advances. Robots designed to work alongside humans in settings such as hospitals, homes, or factories must be able to understand and respond to human gestures, speech, and behavior. AI-powered natural language processing (NLP) algorithms enable robots to communicate with humans and follow verbal instructions, improving their usability and safety in shared environments.

Swarm robotics

Swarm robotics is an emerging field that draws inspiration from natural systems, such as ant colonies or bird flocks, where large numbers of simple agents work together to achieve complex goals. AI and ML are being used to design control algorithms that enable robots to collaborate in swarms, coordinating their actions to perform tasks like search and rescue, environmental monitoring, or space exploration. In swarm robotics, each robot operates autonomously, but AI algorithms allow them to communicate and coordinate their actions to achieve a collective goal. For example, NASA is exploring swarm robotics for space missions, where multiple small robots could work together to explore planetary surfaces, gather data, and assemble structures.

Challenges and ethical considerations

While AI and ML are driving significant advancements in engineering and robotics, they also raise important challenges and ethical considerations. One of the key challenges is ensuring the safety and reliability of AI-powered systems, particularly in applications like autonomous vehicles, where failures can have life-threatening consequences. Ensuring that these systems are robust and can handle unexpected situations is a critical area of research. Data privacy and security are also important concerns, especially in AI-driven smart systems that collect and analyze large amounts of data. Ensuring that sensitive data is protected and that AI systems are not vulnerable to cyber attacks is essential for maintaining trust in these technologies. Finally, there are ethical questions related to the impact of automation on employment. As AI and robots take on more tasks traditionally performed by humans, industries will need to address the potential displacement of workers and the social and economic implications of widespread automation.

AI and ML are revolutionizing the fields of engineering and robotics, providing powerful tools to optimize design, improves maintenance and enables the creation of intelligent, autonomous systems. These technologies are accelerating innovation across a wide range of engineering disciplines, from mechanical and civil engineering to electronics and robotics. As AI and ML continue to evolve, they will play an increasingly important role

in shaping the future of industry, infrastructure, and human-robot interaction, while also presenting new challenges and ethical considerations that must be addressed.

Additive manufacturing (3D Printing)

Additive manufacturing, commonly known as 3D printing is another area where AI and ML are making significant contributions (PostProcess Technologies, 2023). AI can optimize the design and printing process by predicting how different materials will behave during manufacturing and adjusting the parameters accordingly. This ensures the production of high-quality parts with minimal waste. In addition to improving the printing process itself, AI-driven design tools enable engineers to create complex geometries that were previously impossible to manufacture. Generative design, an AI-driven approach, allows engineers to input their design goals (such as weight reduction or structural integrity), and the AI generates multiple designs that meet these criteria. This process has been used in industries such as aerospace and automotive to produce lightweight, durable parts that improve fuel efficiency and reduce costs. Additive Manufacturing has transformed the way products are designed and manufactured. It allows the production of complex geometries, customization, and rapid prototyping, which are impossible or costly with traditional manufacturing methods. The incorporation of Artificial Intelligence (AI) and Machine Learning (ML) into additive manufacturing has opened up new possibilities, optimizing the process, improving material properties, and enabling smarter machines. This chapter explores how AI and ML are being applied in the different stages of additive manufacturing, from design and process optimization to quality control and production automation.

AI and ML in design for additive manufacturing

The design phase is one of the most critical aspects of additive manufacturing. AI and ML have brought new methodologies for design optimization, ensuring that the final product is both structurally efficient and cost-effective to produce. In traditional design processes, engineers must manually iterate on designs to meet both functional and manufacturing requirements, which is time-consuming and often suboptimal. With AI and ML, this process becomes automated and more efficient.

Generative design

One of the most revolutionary AI applications in design for additive manufacturing is generative design. This method uses AI algorithms to generate design alternatives based on specific performance criteria, such as weight reduction, structural integrity, or thermal

management. These designs are typically optimized for 3D printing and often result in organic, non-intuitive structures that maximize material efficiency. Generative design software, such as Autodesk's Fusion 360 or Siemens NX, allows engineers to input design constraints (e.g., material properties, loading conditions), and the AI algorithms generate a multitude of optimized designs. The process saves time and ensures the most effective use of materials. AI's ability to simulate and analyze design iterations rapidly enables faster time to market for new products.

Topology optimization

AI-driven topology optimization is another important tool in 3D printing. In this approach, AI algorithms remove unnecessary material from a part while ensuring that the final structure still meets functional requirements like strength and durability. This leads to lightweight structures that consume fewer resources during production. For instance, General Electric (GE) uses AI for topology optimization in the design of aircraft components, reducing weight by up to 40% while maintaining structural integrity. These designs are crucial in industries like aerospace, where weight reduction directly translates into lower fuel consumption and increased efficiency.

Process optimization in additive manufacturing

One of the primary challenges in additive manufacturing is ensuring consistent quality across printed parts, particularly when dealing with complex geometries or advanced materials. AI and ML can be used to optimize the printing process, improving speed, accuracy, and material performance.

Print parameter optimization

The additive manufacturing process involves a wide range of parameters, such as laser power, print speed, layer thickness, and material flow rates. Traditionally, adjusting these parameters for optimal results requires trial and error, which can be costly and time-consuming. With AI and ML, manufacturers can optimize these parameters in real-time by analyzing data collected from sensors during the printing process. For example, ML algorithms can analyze large datasets from previous print jobs to predict the optimal combination of parameters for a given design. This leads to improved surface finish, dimensional accuracy, and overall print quality. AI-driven optimization tools like 3D Optimize allow for precise tuning of parameters, reducing waste and improving efficiency.

Process control and monitoring

AI-based process control systems ensure that 3D printers operate at peak efficiency, constantly adjusting parameters during printing to account for variations in material behavior, machine wear, or environmental conditions. In-situ monitoring systems, powered by ML, collect data from sensors (e.g., cameras, temperature gauges, and lasers) to ensure that the print process is proceeding as expected. Anomalies, such as overheating, material deposition errors, or warping, can be detected early through AI-powered systems. Real-time process control allows manufacturers to halt printing or make corrections mid-process, reducing defects and improving the success rate of printed parts. For example, AI-driven monitoring systems from companies like Sigma Labs and Stratasys use machine learning to detect anomalies during the metal additive manufacturing process, ensuring higher reliability for critical applications like aerospace and medical devices.

AI and ML for material development

In additive manufacturing, material properties are critical to the performance of the final product. AI and ML are accelerating the discovery and optimization of materials used in 3D printing by analyzing vast amounts of data to predict material behavior, performance, and compatibility with various manufacturing processes.

Materials discovery

Machine learning techniques are being applied to the discovery of new materials for additive manufacturing. Traditionally, material development involved extensive experimentation to test different combinations of elements and manufacturing techniques. With AI, researchers can use data-driven models to predict material properties, such as strength, thermal resistance, or flexibility, without the need for extensive physical testing. For instance, researchers at Lawrence Livermore National Laboratory are using AI to predict the behavior of new polymer resins used in 3D printing. By training ML models on existing material datasets, they can predict the best material formulations for specific applications, such as medical implants or high-strength aerospace parts.

Material behavior prediction

Understanding how materials will behave during the printing process is a major challenge in additive manufacturing. AI and ML models can predict thermal distortion, shrinkage, or warping of materials during and after printing, allowing for proactive adjustments in print strategies. These predictions improve both the dimensional accuracy and mechanical performance of parts. For example, in metal additive manufacturing, where

precise control over the cooling rates and solidification process is crucial, ML models can predict how different alloys will behave under specific conditions. This allows manufacturers to adjust print parameters to avoid defects like porosity or cracking.

Quality assurance and defect detection

Quality control in additive manufacturing is vital, especially in industries where high performance and safety are critical, such as aerospace, automotive, and healthcare. AI and ML play a significant role in improving defect detection and ensuring consistent part quality across production runs.

Automated inspection systems

AI-powered automated inspection systems are used to analyze 3D-printed parts for defects, such as cracks, porosity, or dimensional inaccuracies. Traditionally, inspection is done manually or through non-destructive testing methods like X-ray or CT scanning, which can be slow and costly. AI systems can quickly process data from these scans and identify defects with greater accuracy and speed. For example, AI systems developed by companies like GE Additive use machine learning to analyze data from industrial X-rays, detecting defects in metal parts printed through additive manufacturing. These systems not only reduce inspection time but also provide more reliable detection, ensuring that critical parts meet stringent quality standards.

Predictive quality models

Machine learning can also be used to build predictive models that anticipate the likelihood of defects based on the data collected during the printing process. These models help manufacturers identify process conditions that are likely to produce defects and adjust the process in real time to avoid them. This reduces waste, improves yield, and lowers the overall cost of production. In industries like bioprinting, where printed structures must meet precise biological and mechanical standards, ML algorithms are used to predict how well a print will meet these standards based on material composition, environmental conditions, and printer settings.

AI-driven automation in additive manufacturing

The integration of AI and ML is paving the way for fully automated additive manufacturing systems that can operate with minimal human intervention. These systems enable lights-out manufacturing, where machines run continuously without direct oversight, maximizing productivity and reducing costs.

Intelligent scheduling and workflow automation

AI-driven workflow management systems automate the scheduling of print jobs, ensuring that machines are used efficiently. ML algorithms optimize the order in which parts are printed, balancing factors such as machine availability, material requirements, and deadlines. This reduces downtime and ensures that production schedules are met with minimal delays. For example, in industries like automotive manufacturing, where large numbers of parts must be produced on tight schedules, AI-powered scheduling systems can automatically adjust print queues based on real-time data from the production floor.

Robotic integration and post-processing automation

Additive manufacturing often requires post-processing steps, such as support removal, surface finishing, or heat treatment. AI-powered robots are increasingly being integrated into 3D printing workflows to automate these tasks. Robotic arms, guided by AI vision systems, can perform precise post-processing operations on printed parts, reducing the need for manual labor and increasing throughput. Companies like PostProcess Technologies are developing automated post-processing solutions that use AI to optimize the finishing process based on the geometry and material of the printed part. This ensures consistent quality and reduces the time and cost associated with manual post-processing.

Challenges and future directions

Despite the significant advancements in AI and ML for additive manufacturing, several challenges remain. One major hurdle is the lack of standardized data across different 3D printing processes and materials, making it difficult to build generalizable AI models. Additionally, the integration of AI into existing manufacturing workflows requires significant investment in hardware, software, and training. Looking forward, the combination of AI, ML, and additive manufacturing holds great promise for industries ranging from aerospace and healthcare to consumer goods and electronics. As AI algorithms become more sophisticated and 3D printing technology continues to evolve, fully autonomous, AI-driven manufacturing systems are likely to become the norm, revolutionizing how products are designed, produced, and delivered.

AI and ML are fundamentally transforming additive manufacturing by enabling smarter design, process optimization, material innovation, and quality assurance. These technologies are driving the evolution of 3D printing from a prototyping tool to a mainstream manufacturing process capable of producing high-quality, customized products at scale. The integration of AI into additive manufacturing systems is not only

enhancing productivity and efficiency but also unlocking new possibilities for innovation in product design, material science, and manufacturing automation.

Artificial intelligence and machine learning in climate science and environmental research

The application of AI and ML in climate science is helping researchers understand and address one of the most significant challenges of the 21st century: climate change. These technologies are used to analyze massive datasets collected from satellites, weather stations, and ocean sensors, enabling scientists to model climate systems and predict future climate scenarios with greater accuracy. For instance, AI models are used in climate modeling to simulate the Earth's climate system, including interactions between the atmosphere, oceans, and land surfaces. These models help researchers predict the impacts of climate change on weather patterns, sea-level rise, and biodiversity. One prominent example is the CMIP6 project, which uses machine learning algorithms to improve the accuracy of climate predictions by analyzing historical climate data. AI is also being used to develop solutions for sustainable energy. Machine learning algorithms optimize the operation of renewable energy systems, such as wind turbines and solar panels, by predicting energy production based on weather conditions. This enables more efficient energy storage and distribution, helping to integrate renewable energy into the grid and reduce reliance on fossil fuels.

Artificial Intelligence and Machine Learning have increasingly become integral tools in climate science and environmental research. These advanced technologies can process large datasets, make predictions; identify patterns, and model complex systems that are beyond the capabilities of traditional methods. By leveraging AI and ML, researchers can address some of the most pressing environmental challenges, from climate modeling and weather forecasting to managing ecosystems and predicting the impacts of climate change. Below is a detailed exploration of the roles that AI and ML play in these fields, along with relevant applications, benefits, challenges, and future prospects.

Artificial intelligence and machine learning in climate modeling

Climate models are essential for predicting future climate scenarios, understanding how human activities affect the climate system, and guiding policy decisions. Traditional climate models, known as General Circulation Models (GCMs), rely on physical equations to simulate interactions between the atmosphere, oceans, and land. However, these models have limitations, including computational intensity and the challenge of accurately

capturing regional climate dynamics. AI and ML offer alternative approaches to climate modeling by improving both the accuracy and efficiency of predictions.

Data-driven climate models: ML algorithms can be trained on historical climate data to make predictions about future climate states. These data-driven models can reduce the need for high-computational resources associated with physics-based models.

Downscaling global models: GCMs often work at coarse resolutions, making it difficult to predict local and regional climate impacts. AI techniques like convolutional neural networks (CNNs) can be used to downscale these models, providing high-resolution regional climate forecasts.

Climate sensitivity analysis: Estimating climate sensitivity, the degree to which temperatures increase in response to greenhouse gas emissions, is crucial for understanding long-term climate impacts. AI can accelerate the computation of various climate sensitivity scenarios, offering faster insights into how different variables interact in the climate system.

Weather forecasting: Weather forecasting is one of the earliest areas to benefit from AI and ML. Traditional numerical weather prediction (NWP) models are based on physical principles and are limited by computing power and the resolution of data. AI has been instrumental in addressing these challenges:

Nowcasting: AI, particularly deep learning models like Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks, have been used for short-term weather predictions or "nowcasting," which involves predicting weather on the scale of hours. This is particularly useful for predicting extreme events like thunderstorms, flash floods, or hurricanes.

Data assimilation: AI can enhance the assimilation of diverse data sources (e.g., satellite, radar, and ground stations) to improve the accuracy of weather forecasts. For example, generative adversarial networks (GANs) have been applied to fill gaps in satellite imagery or radar data, enhancing forecast models.

Seasonal predictions: AI can improve seasonal weather forecasts by integrating historical patterns with real-time data. ML algorithms, such as support vector machines (SVMs) and random forests, can analyze complex patterns in ocean-atmosphere interactions, such as the El Niño Southern Oscillation (ENSO), to predict seasonal climate anomalies like droughts or monsoons.

Environmental monitoring and ecosystem management

AI and ML have also become vital tools in monitoring the environment, from tracking deforestation and air pollution to managing ecosystems and biodiversity. These technologies are transforming how scientists gather and interpret data to make more informed environmental decisions.

Remote sensing and satellite imagery: AI-based techniques like deep learning are now applied to analyze remote sensing data from satellites. AI can automatically classify land use changes, detect illegal logging, monitor forest health, and track pollution levels. This automated analysis allows researchers to process vast amounts of data quickly and efficiently, aiding in large-scale environmental monitoring.

Wildlife conservation: ML techniques are increasingly being used to analyze animal movement patterns and habitat use. For example, neural networks can be used to process camera trap images, identifying species automatically. Additionally, drones equipped with AI can be used to monitor endangered species, detect poaching, and manage protected areas.

Water resource management: AI and ML are also being used to predict water quality, manage reservoirs, and optimize irrigation. ML algorithms like random forests and gradient boosting are helping predict harmful algal blooms, assess water contamination, and ensure sustainable water resource management.

AI in carbon management and climate mitigation: AI is playing a critical role in climate mitigation by optimizing energy use, reducing carbon emissions, and managing renewable energy sources.

Energy optimization: AI models can optimize energy consumption in industries and households. For example, Google has used AI to reduce energy consumption in its data centers by as much as 40% by optimizing cooling systems.

Carbon sequestration: AI is being used to optimize carbon capture and storage (CCS) technologies by predicting the most effective methods for capturing CO2 and identifying suitable storage locations.

Renewable energy forecasting: AI is also improving the integration of renewable energy into the grid by forecasting energy production from solar and wind farms. By predicting weather patterns and energy demand, AI can help balance energy supply and demand, improving the reliability of renewable energy systems.

Challenges and ethical considerations:

While AI and ML offer immense promise in climate science and environmental research, they come with several challenges:

Data availability and quality: Many AI and ML models require large, high-quality datasets, which are not always available in climate science, particularly in developing regions. Gaps in data coverage can limit the accuracy and applicability of AI-driven models.

Computational resources: AI models can be computationally expensive, particularly deep learning techniques. This can limit their accessibility, especially for researchers in less-resourced institutions or countries.

Ethical concerns: AI models can inadvertently exacerbate environmental justice issues. For instance, energy optimization in urban areas might disproportionately benefit wealthier communities while neglecting low-income neighborhoods, reinforcing social inequalities. Additionally, AI-based environmental surveillance, such as drones or automated monitoring, could infringe on privacy rights and raise ethical concerns.

Future prospects

The future of AI and ML in climate science and environmental research holds exciting possibilities:

Interdisciplinary integration: Future advancements in AI will likely require interdisciplinary collaboration between climate scientists, computer scientists, and ethicists. This collaboration will ensure that AI models are not only scientifically robust but also socially responsible.

AI-augmented climate policy: AI has the potential to shape climate policy by providing data-driven insights into the most effective climate mitigation strategies. By modeling complex interactions between economic activities, energy systems, and environmental policies, AI can guide decision-makers in designing more effective policies.

Emerging technologies: Advances in quantum computing, along with more sophisticated AI models could revolutionize climate modeling, making it possible to simulate the climate system with unprecedented accuracy and speed.

AI and ML are reshaping climate science and environmental research, offering powerful tools for predicting, monitoring, and mitigating environmental changes. From improving climate models to optimizing renewable energy systems and conserving biodiversity, AI is poised to play an even more prominent role in addressing the global environmental challenges of the 21st century. However, realizing the full potential of these

technologies will require addressing challenges related to data availability, computational resources, and ethical considerations. As AI continues to advance, its integration with climate science will be critical in driving both scientific discovery and sustainable environmental solutions.

Challenges and ethical considerations

While AI and ML offer enormous potential in scientific research, they also pose significant challenges. One of the primary concerns is the interpretability of AI models. Many AI systems, particularly deep learning models, are often described as "black boxes" because it is difficult to understand how they arrive at their conclusions. This lack of transparency can be problematic, particularly in fields such as medicine, where decisions made by AI systems can have life-or-death consequences. Ethical considerations are also paramount, particularly regarding data privacy and bias. AI systems trained on biased datasets can perpetuate inequalities, leading to biased outcomes in areas such as healthcare, criminal justice, and hiring. Ensuring that, AI models are fair, transparent and accountable is a key challenge that researchers must address as these technologies continue to evolve.

Conclusion:

Artificial Intelligence and Machine Learning are reshaping the landscape of scientific research, providing tools that enable faster, more efficient discovery across a wide range of disciplines. From accelerating drug discovery and improving medical diagnostics to predicting climate change and designing new materials, AI and ML are driving innovation at an unprecedented pace. As researchers continue to refine these technologies and address the ethical challenges they pose, AI and ML will remain integral to the future of science and technology research, unlocking new frontiers in human knowledge. The integration of Artificial Intelligence and Machine Learning into research is revolutionizing the way scientists approach discovery, problem-solving, and innovation. Throughout this chapter, we have explored how these technologies are transforming diverse fields, from materials science to biomedicine, chemistry, physics, and climate science, by accelerating data processing, enhancing predictive accuracy, and facilitating the exploration of complex systems that were once considered too intricate for traditional methods.

The primary advantage of AI and ML lies in their capacity to process vast datasets with speed and precision, uncovering patterns, relationships, and insights that are often imperceptible to human researchers. This capability has not only accelerated the pace of

discovery but also broadened the horizons of scientific inquiry, enabling the design of more efficient experiments and the development of novel hypotheses. The success of AI in fields like materials discovery, drug design, and climate modeling underscores the potential of these technologies to address some of the most pressing challenges facing humanity, including sustainable energy solutions, personalized healthcare, and climate change mitigation. While AI and ML have proven their value, this chapter has also highlighted several key challenges and limitations. Bias in AI models remains a significant concern, particularly when algorithms are trained on unrepresentative or incomplete datasets. The ethical implications of AI-driven decisions, particularly in fields like healthcare and drug discovery, demand careful consideration to ensure fairness and inclusivity. Efforts to create explainable AI—systems that provide transparency in their decision-making processes—will be critical in building trust and ensuring responsible use of AI technologies in scientific research. Looking forward, the future of AI and ML in research is filled with promise. These technologies will likely continue to evolve, offering even more sophisticated tools for tackling complex scientific questions. Emerging trends such as AI-enhanced experimental design, automated hypothesis generation and AI-driven simulations are poised to further push the boundaries of what is scientifically possible. As computational power increases and new algorithmic techniques emerge, AI's role in augmenting human ingenuity will only deepen, reshaping the scientific landscape and driving innovation across disciplines. The next phase of AI in research will likely see a deeper integration of human and machine collaboration, where AI augments human creativity and insight rather than replacing it. Researchers will increasingly rely on AI to process and interpret the overwhelming volumes of data generated by modern experimental techniques, enabling more informed and creative scientific exploration. Moreover, as AI systems become more adaptable and intelligent, the line between theoretical research and experimental implementation may blur, leading to a new paradigm of closed-loop research, where AI continually refines and adapts experimental processes based on real-time data. In conclusion, AI and ML have already begun to redefine the boundaries of scientific research, offering tools that are not just accelerators of existing processes but drivers of entirely new forms of inquiry. While challenges around bias, ethics, and transparency remain, the potential for AI to augment human capabilities and foster groundbreaking discoveries is undeniable. As AI technologies continue to mature, they will play an increasingly integral role in shaping the future of scientific discovery, providing researchers with the tools they need to tackle some of the

most complex and urgent problems of our time. The promise of AI and ML in research is vast, and their full potential is only beginning to be realized.

Acknowledgments

We are very much thankful to the authors of different publications as many new ideas are abstracted from them. The authors are highly thankful to Bhumi Publishing for providing the opportunity to publish this book chapter. Authors also express gratefulness to their colleagues and family members for their continuous help, inspirations, encouragement, and sacrifices without which the book chapter could not be executed. Finally, the main target of this book will not be achieved unless it is used by research institutions, students, research scholars, and authors in their future works. The authors will remain ever grateful to Dr. H. S. Ginwal, Director, ICFRE-Tropical Forest Research Institute, Jabalpur who helped by giving constructive suggestions for this work. The authors are also responsible for any possible errors and shortcomings, if any in the book, despite the best attempt to make it immaculate.

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HARNESSING THE POWER OF ENSEMBLES: ADVANCED TECHNIQUES IN RECOMMENDER SYSTEMS

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Abstract:

Ensemble methods have emerged as a crucial advancement in recommender systems by combining multiple models to boost prediction accuracy and decision-making processes. This chapter introduces the fundamental concepts of ensemble-based recommenders, followed by an exploration of techniques like bagging, boosting, and stacking, which enhance recommendation robustness. It discusses the methodology for constructing ensemble systems, including the selection of base models, combining their predictions, and optimizing them for various applications. Empirical evaluations compare ensemble approaches with traditional recommenders, highlighting improvements in accuracy, diversity, and scalability. Real-world case studies showcase the benefits and challenges of implementing these systems. The chapter concludes by addressing future directions, emphasizing the potential of integrating deep learning and AI, as well as the challenges of computational complexity and adaptive algorithms for evolving user preferences.

Keywords: Ensemble Learning; Recommendation System; Bagging; Boosting; Accuracy.

1. Introduction:

Ensemble-Based Recommender Systems utilize ensemble learning techniques to combine predictions from multiple models, enhancing the quality, accuracy, and robustness of recommendations [1]. Methods like Bagging, Boosting, and Stacking improve prediction accuracy by mitigating overfitting and aggregating diverse sources of information. Studies, such as those by Liu and Aloraini, have shown that these systems can boost recommendation performance and user satisfaction [2-3]. Meta-learning algorithms are often used to combine the strengths of individual models, leading to more stable recommendations. Additionally, diversity-promoting techniques in ensembling, such as varying initializations or feature representations, improve recommendation coverage and serendipity. Bagging reduces variance by training multiple models in parallel on different

data subsets, while Boosting iteratively corrects errors, improving accuracy over time by focusing on misclassified instances. Stacking combines predictions from multiple models through a meta-model, enhancing accuracy by leveraging the strengths of each model. Weighted Models further refine this process by assigning different weights to base models based on their performance, allowing dynamic adjustment of the ensemble's output for better prediction quality. These techniques collectively improve recommender systems by reducing biases, improving adaptability, and offering personalized recommendations. As a result, ensemble learning has become a cornerstone in advancing recommendation technology, helping systems better cater to user needs in a dynamic environment [4].

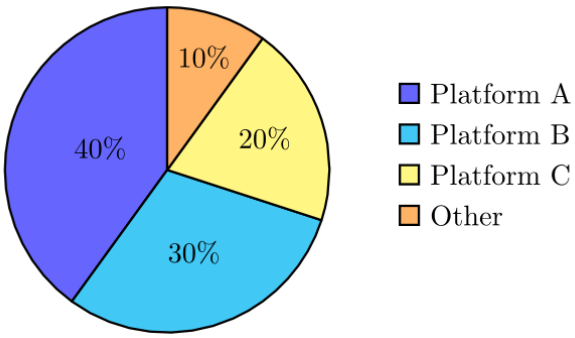

Figure 1: Stimulation Platforms for Ensemble-based Recommender Systems

2. Methodology used in different techniques of ensemble learning

2.1 Homogeneous ensemble learning methods

Homogeneous ensemble learning methods involve combining multiple models of the same type to improve predictive performance. The most common techniques in this category include bagging, boosting, and stacking [5]. In bagging (Bootstrap Aggregating), multiple instances of the same model are trained on different subsets of the data created through random sampling with replacement. This method helps to reduce variance and avoid overfitting. A well-known example of bagging is the Random Forest algorithm, which builds an ensemble of decision trees. Each tree in a Random Forest is trained on a random subset of features and samples, leading to diverse trees that contribute to a more robust final model. Boosting, on the other hand, sequentially trains the same model type, where each new model attempts to correct the errors made by the previous models. AdaBoost and Gradient Boosting are popular boosting techniques that enhance model accuracy by focusing on difficult-to-predict instances [6-7]. In boosting, models are weighted based on their accuracy, with more emphasis placed on correcting the mistakes of the weaker models. This sequential focus can lead to significant improvements in model performance.

In stacking, multiple homogeneous models are trained, and their predictions are used as input features for a higher-level model, which is often a simple linear model or another complex algorithm, to make the final prediction. Stacking can significantly improve predictive performance by combining the strengths of multiple models.

2.1.1 Bagging (Bootstrap aggregating)

Bagging, or Bootstrap Aggregating, stands as a cornerstone in ensemble learning, a powerful technique used to bolster model stability and mitigate the risk of overfitting in machine learning tasks [8]. At its core, bagging operates by training multiple models, often referred to as base or weak learners, on different subsets of the original dataset. These subsets, known as bootstrap samples, are generated through random sampling with replacement from the original data pool. This strategic sampling ensures that each instance in the dataset has an equal chance of being selected for inclusion in a given subset. This process of bootstrapping allows each model to glean insights from a unique perspective of the data, thus fostering diversity within the ensemble. By exposing the models to distinct variations of the dataset, bagging minimizes the ensemble's reliance on any particular idiosyncrasy or noise present in the data [9-10]. Consequently, it leads to a more robust and generalized final model, capable of making accurate predictions on unseen data.

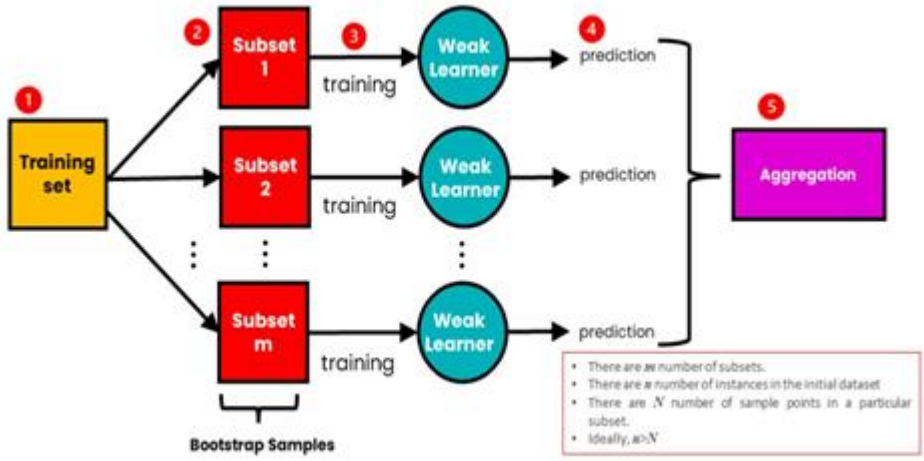

Figure 2: Bagging Ensemble Method

2.1.2 Boosting

Boosting represents a sophisticated approach within the ensemble learning framework, characterized by its iterative nature and emphasis on gradually refining the ensemble's predictive capabilities [11]. Unlike bagging, which trains each base model independently, boosting incrementally constructs the ensemble by training new models to rectify errors made by the previously trained ones. This iterative process focuses on

instances that are more challenging to predict, effectively adjusting the data distribution to prioritize the most difficult cases. By repeatedly emphasizing the misclassified samples in subsequent iterations, boosting enables the ensemble to gradually improve its performance, particularly in regions of the feature space where the models struggle to make accurate predictions. One of the hallmark features of boosting is its ability to assign performance-based weights to each model in the ensemble. Models that demonstrate higher accuracy or contribute more substantially to reducing prediction errors are assigned greater influence in the final composite outcome [12-13].

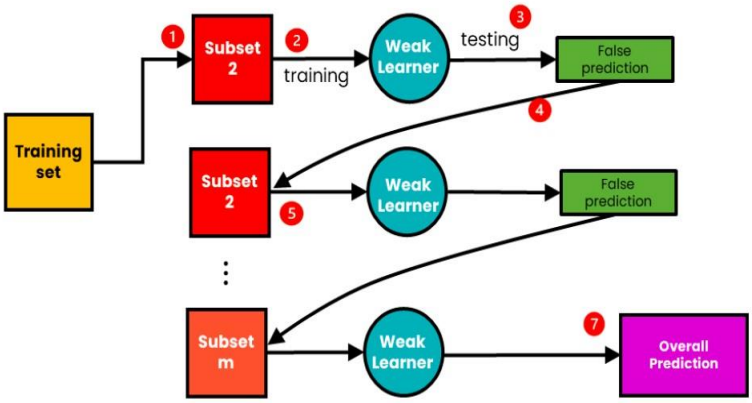

Figure 3: Boosting Ensemble Method

This weighting scheme ensures that more accurate predictors exert a stronger influence on the ensemble's decision-making process, effectively guiding it towards improved performance. Consequently, boosting algorithms such as AdaBoost dynamically adjust the importance of each base model based on its performance, allowing the ensemble to adapt and prioritize the most informative models throughout the iterative training process. Overall, boosting stands as a sophisticated and powerful ensemble technique that leverages the strengths of multiple models to enhance predictive performance. By iteratively refining the ensemble through focused attention on challenging instances and dynamically adjusting model weights based on performance, boosting algorithms achieve remarkable predictive accuracy across a wide [14]. Boosting is effective at reducing bias and enhancing the predictive performance of relatively simple models, making it a robust choice for improving underfitting base learners.

2.2 Heterogeneous ensemble learning methods

Heterogeneous ensemble learning methods combine different types of models to leverage the strengths and compensate for the weaknesses of each model type. This approach is particularly useful when diverse algorithms capture different patterns or

structures in the data [15]. A common method in heterogeneous ensembles is stacking, where models of various types (e.g., decision trees, support vector machines, neural networks) are trained on the same dataset, and their predictions are fed into a meta-model that synthesizes these predictions into a final output. For instance, a heterogeneous ensemble might include a decision tree to capture non-linear relationships, a support vector machine for high-dimensional data, and a neural network for complex pattern recognition. Another approach is voting, where different models cast votes for each class label, and the final prediction is determined by majority or weighted voting [16]. This method is straightforward and often improves accuracy by averaging out the biases and variances of individual models. For example, a simple majority vote could be used where each model's prediction is equally weighted, or a weighted vote could be employed where more accurate models have a greater influence on the final prediction. Blending is similar to stacking but involves combining predictions in a weighted or linear manner without a separate meta-model. Blending typically uses holdout validation sets to determine the best way to combine the predictions. Heterogeneous ensembles often result in more robust and accurate models, as they integrate the diverse strengths of different algorithms, capturing a wider range of patterns and reducing the risk of overfitting to any single model's biases.

2.2.2.1 Stacking

Stacking involves using a meta-learner or meta-model to optimally combine predictions from multiple base models. The base models are first trained on the full dataset, and then their predictions are used as input features for the meta-learner. This second-stage model learns how to best integrate these diverse inputs to form a final prediction:

$$R_{stack}(u,i) = g(R1(u,i), R2(u,i), \ldots\ldots\ldots RT(u,i)$$

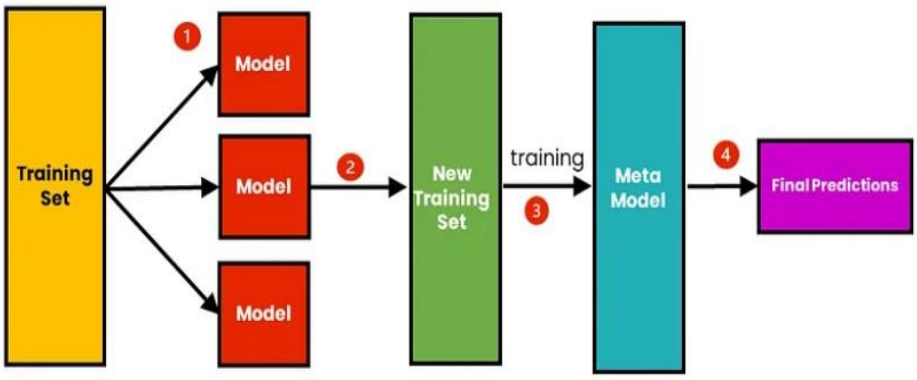

Figure 4: Stacking Ensemble Method

where g represents the meta-learner. The meta-learner is typically a different type of model or algorithm than the base models, chosen specifically for its ability to synthesize information effectively. This method leverages the heterogeneity of the base models to capture a broad spectrum of patterns and relationships in the data, often resulting in superior predictive performance [17]. Along with these ensemble methods, there are several additional one's worth mentioning. These include methods such as Majority Voting, Averaging, Weighted Averaging *etc.*

2.2.2 Majority Voting

Max voting, or majority voting, is a simple yet powerful ensemble method commonly employed in classification tasks. It leverages the principle of combining the predictions from multiple base classifiers to achieve a final prediction with improved accuracy and reliability. In the max voting ensemble, each base classifier Ci independently predicts the class label for a given input sample. Let's denote the set of possible class labels as L, where |L| represents the total number of unique class labels. For a particular input sample, each classifier Ci produces a probability distribution over the class labels. Let pij denote the probability assigned by classifier Ci to class label j. These probabilities can be obtained through methods like softmax in neural networks or probability estimates in decision trees.

The final prediction y is then determined by selecting the class label that receives the most "votes" from the individual classifiers. Mathematically, this is represented as:

$$y = \arg\max_{j \in L} \sum_{i=1}^{n} 1(C_i = j)$$

Here, 1(.) is the indicator function, which equals 1 if the condition inside the parentheses is true and 0 otherwise. Essentially, for each class label j, we sum up the number of classifiers that predict j as the class label. The class label with the highest sum of votes across all classifiers is selected as the final prediction y. Max voting is appealing due to its simplicity and effectiveness. It allows diverse classifiers, each potentially capturing different aspects of the data, to contribute to the final decision. By aggregating the predictions of multiple classifiers, max voting tends to reduce overfitting and variance, leading to more robust predictions. However, max voting may encounter challenges when dealing with imbalanced datasets or when classifiers produce highly confident but incorrect predictions. In such cases, more sophisticated ensemble methods like weighted voting or stacking may be employed to address these issues. Overall, max voting serves as a

fundamental ensemble technique in classification tasks, providing a straightforward yet reliable approach to harnessing the collective intelligence of multiple classifiers.

2.2.3 Weighted averaging

Weighted averaging is an ensemble method used primarily in regression tasks, although it can also be adapted for classification. In this method, predictions from multiple base models are combined by assigning different weights to each model's prediction [18]. These weights reflect the relative importance or confidence of each model's prediction. Let's denote yi as the prediction made by the i th base model, and wi as the weight assigned to that model's prediction. The weighted average prediction y is then calculated as:

$$y = \sum_{i=1}^{n} w_i \cdot y_i$$

The weights wi can be predetermined based on prior knowledge or determined through techniques such as cross-validation. In regression tasks, it's common to use the inverse of the mean squared error (MSE) or R-squared values of each model as weights, where models with lower errors or higher R-squared values receive higher weights. For classification tasks, soft max function outputs or probability estimates produced by each base model can be used as inputs to calculate the weighted average. The final class label can then be determined by applying a threshold or by selecting the class with the highest probability after normalization [19-20]. Weighted averaging offers flexibility in combining predictions from multiple models. Models that perform better on certain subsets of data or capture different aspects of the problem can be given higher weights, while less reliable models can be assigned lower weights. This allows for the creation of an ensemble that leverages the strengths of individual models while mitigating their weaknesses. However, determining the optimal weights can be challenging and may require experimentation or fine-tuning through techniques like grid search or optimization algorithms. Additionally, weighted averaging may be sensitive to outliers or poorly performing models, which can affect the overall performance of the ensemble. Overall, weighted averaging is a versatile ensemble method that provides a principled approach to combining predictions from multiple models, offering potentially improved performance over individual models alone.

2.2.4 Averaging ensemble method

Averaging ensemble methods, also known as simple averaging, involve combining predictions from multiple base models by taking the arithmetic mean of their predictions [21]. This approach is commonly used in regression tasks, although it can also be adapted

for classification. In averaging ensemble methods, let yij denote the prediction made by the i th base model for the j th sample in the dataset, where i = 1, 2, ..., n represents the index of the model and j = 1, 2, ..., m represents the index of the sample. The average prediction yj for the j th sample is calculated as:

$$y_j = \frac{1}{n} \sum_{i=1}^{n} y_{ij}$$

Here, n represents the total number of base models contributing to the ensemble. For regression tasks, the average prediction yj represents the expected value or mean prediction across all base models for the j th sample. This averaging process aims to reduce variance and improve generalization by leveraging the collective knowledge of multiple models.

In the case of classification tasks, averaging ensemble methods can be adapted to handle class probabilities or scores produced by the base models. For each class label k, the average class probability pkj for the j th sample can be computed as:

$$p_{kj} = \frac{1}{n} \sum_{i=1}^{n} p_{kij}$$

where pkij represents the probability assigned to class label k by the i th base model for the j th sample. After computing the average probabilities pkj for each class label k, the final class label for the j th sample can be determined using methods such as maximum likelihood estimation or by selecting the class label with the highest average probability.

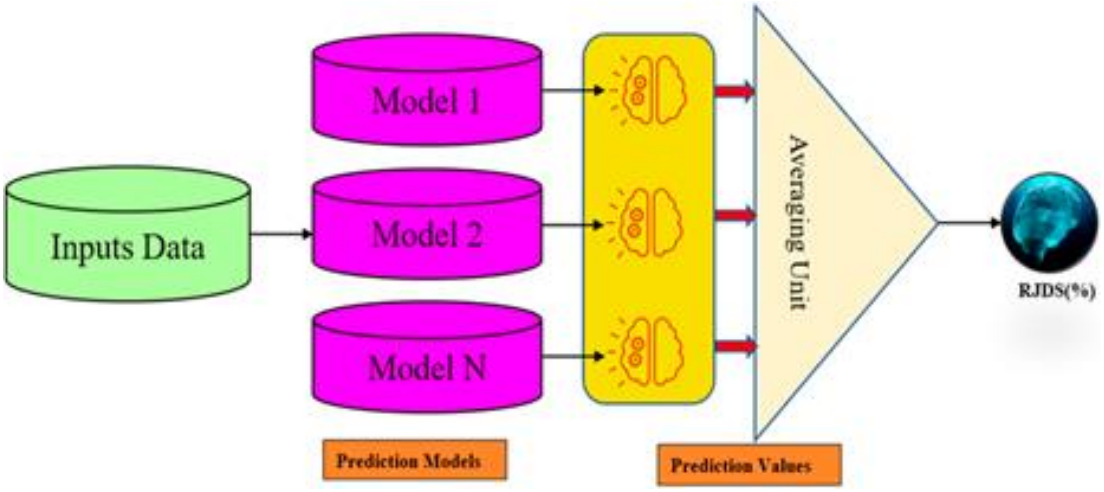

Figure 7: Averaging Ensemble Method

Table 1: Ensemble Configuration Table

Ensemble Configuration	Base Recommender Algorithms	Aggregation Method	Hyperparameters	References
Weighted Average Ensemble	Collaborative Filtering, Content-Based Filtering	Weighted averaging based on performance or expertise	Weight coefficients for each base recommender	[22-23]
Stacking Ensemble	Matrix Factorization, Neural Collaborative Filtering	Meta-learner (e.g.,linear regression, neural network) trained on outputs of base recommenders	Meta-learner architecture, number of layers, activation functions	[24-25]
Bagging Ensemble	Singular Value Decomposition (SVD), Item-based Collaborative Filtering	Bootstrap aggregating (bagging) with majority voting or averaging	Number of base recommenders sampled, bootstrap sample size	[26-27]
Boosting Ensemble	Factorization Machines, LightFM	Sequential boosting (e.g., AdaBoost, Gradient Boosting)	Number of boosting iterations, learning rate, base learner	[28-29]

3. Applications of ensemble methods in different areas

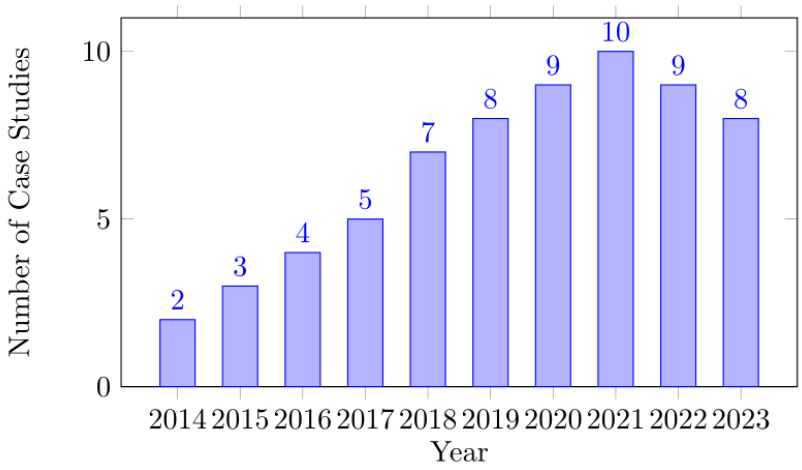

Figure 8: Case Studies of Ensemble-based Recommender Systems Over the Last 10 Years

Table 2: Applications of ensemble methods in different areas

Application Area	Description	Example of Ensemble Methods Used	Key Benefits	References
Finance	Ensemble methods are used for credit scoring to assess the creditworthiness of borrowers, fraud detection to identify suspicious transactions, risk management to predict potential losses, and stock price prediction to forecast future market movements	Random Forest, Gradient Boosting Machines (GBM), Bagging, Voting	Improved accuracy in risk assessments leads to better loan approval decisions; robust fraud detection helps prevent significant financial losses; enhanced investment strategies provide higher returns	[30-31]
Health Care	Used for predicting diseases like diabetes or heart disease, patient readmission prediction to reduce hospital readmissions, analyzing medical images for detecting tumors, and evaluating treatment effectiveness to personalize healthcare plans	Random Forest, AdaBoost, XGBoost, Stacking	Enhanced diagnostic accuracy results in early disease detection; better patient outcomes through tailored treatment plans; personalized healthcare improves patient satisfaction and adherence to treatment	[32-33]
Marketing	Facilitates customer segmentation to tailor marketing strategies, churn prediction to identify customers likely to leave, and evaluating campaign effectiveness to optimize marketing efforts	Gradient Boosting, Random Forest, Voting	More accurate customer insights lead to highly targeted marketing campaigns; improved retention strategies reduce churn rates; optimized marketing spend maximizes return on investment (ROI)	[34-35]

Retail	Applied in demand forecasting to ensure adequate stock levels, recommendation systems to suggest products to customers, and predicting customer lifetime value to inform long-term strategies	XGBoost, Random Forest, Bagging	Improved inventory management reduces stockouts and overstock situations; personalized shopping experiences increase customer satisfaction and sales; increased customer loyalty and lifetime value drive long-term profitability	[36-37]
Tele-communications	Helps in network fault detection to maintain service quality, predicting customer churn to reduce turnover, and managing service quality to enhance customer satisfaction	Random Forest, AdaBoost, Gradient Boosting	Enhanced network reliability minimizes service disruptions; reduced customer churn rates increase revenue; improved service delivery boosts customer satisfaction and loyalty	[38-39]
Manufacturing	Used for predictive maintenance to foresee equipment failures, quality control to detect defects in products, and optimizing the supply chain for efficient resource allocation	Random Forest, Gradient Boosting, Bagging	Reduced operational downtime saves costs and increases productivity; higher product quality leads to fewer returns and recalls; streamlined supply chain management enhances efficiency and reduces waste	[40-41]
Energy	Involves load forecasting to predict energy demand, renewable energy production prediction to optimize resource usage, and fault detection in energy systems to ensure uninterrupted service	Gradient Boosting, Random Forest, Stacking	Better energy management allows for cost savings and sustainability; improved efficiency in renewable energy usage; reliable energy supply minimizes outages and enhances customer satisfaction	[42-43]

E-Commerce	Utilized for personalized product recommendations, segmenting customers based on behavior, and sentiment analysis to understand customer opinions and improve service	XGBoost, Random Forest, Voting	Enhanced customer experience through personalized recommendations; targeted marketing based on accurate customer segmentation; better customer service by understanding and addressing sentiment	[44-45]
Social Media	Applied in sentiment analysis to gauge public opinion, detecting fake news to maintain platform integrity, and predicting user engagement to tailor content delivery	Random Forest, Gradient Boosting, Stacking	Improved content relevance keeps users engaged longer; safer online communities with effective fake news detection; higher user engagement and retention rates through tailored content	[46-47]
Transportation	Used for traffic prediction to manage congestion, vehicle routing to optimize delivery paths, and demand prediction for ride-sharing services to balance supply and demand	Gradient Boosting, Random Forest, AdaBoost	Efficient traffic management reduces congestion and travel times; cost-effective routing saves fuel and time; better service availability meets customer demand effectively	[48-49]
Banking	Involves predicting loan defaults to manage credit risk, detecting fraudulent transactions to protect against financial crimes, and segmenting customers for personalized banking services	Random Forest, Gradient Boosting, Bagging	Reduced financial risk with accurate loan default predictions; enhanced fraud protection safeguards assets and customers; tailored customer services improve satisfaction and retention	[50-51]

Insurance	Used for predicting claims to assess potential payouts, detecting fraudulent claims to prevent losses, and assessing risk for setting insurance premiums	Random Forest, AdaBoost, Gradient Boosting	Improved risk management leads to more accurate premium setting; reduced fraudulent claims lower costs; fairer premium pricing increases customer trust and retention	[52-53]
Education	Facilitates predicting student performance to provide targeted support, dropout prediction to reduce attrition rates, and personalized learning to cater to individual student needs	Random Forest, Gradient Boosting, Stacking	Better academic performance through early intervention; lower dropout rates increase graduation rates; customized learning experiences cater to individual student needs and improve learning outcomes	[54-55]
Real Estate	Applied in predicting property prices to guide buying and selling decisions, analyzing market trends to forecast future developments, and evaluating investments to optimize returns	Gradient Boosting, Random Forest, Voting	More accurate pricing ensures better investment decisions; informed investment choices based on market trends; better market predictions enhance strategic planning	[56-57]
Agriculture	Used for crop yield prediction to plan agricultural activities, pest detection to manage infestations, and soil quality assessment to enhance farming practices	Random Forest, Gradient Boosting, Bagging	Increased agricultural productivity through precise yield predictions; effective pest management reduces crop losses; sustainable farming practices improve soil health and long-term viability	[58-59]

Conclusion:

In conclusion, this chapter has thoroughly examined efficient ensemble-based recommender systems, highlighted their key benefits and outlined future research directions. It explored the mechanisms and methodologies that make these systems effective, focusing on their ability to enhance accuracy, robustness, and diversity in recommendations. By combining multiple base models, ensemble methods reduce biases and utilize diverse information sources, leading to more reliable and personalized recommendations. These systems are crucial in addressing challenges such as data sparsity, cold-start issues, and scalability, improving user satisfaction in today's personalized, data-driven landscape. Looking forward, integrating deep learning, developing personalized strategies, and designing real-time systems are promising areas for further research, which will drive advancements in recommendation technology and user experience. Efficient ensemble-based systems thus serve as a foundational framework for delivering precise and diverse recommendations.

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ERROR FUNCTION

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Introduction:

The error function, often denoted as erf(x) is a fundamental concept in probability and statistics. It arises in various applications, including statistical analysis, heat diffusion problems and in the evaluation of integrals involving Gaussian distribution. This chapter will explore basic part of error function and its properties.

1.Definition: Error function of x is defined as $\frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du$ and is denoted by erf(x)

We write

$$\mathbf{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du$$

This function or integral is also called Error function integral or probability integral and it has applications in many branches of Mathematics and Engineering. The plot of error function for different values of x are as follow.

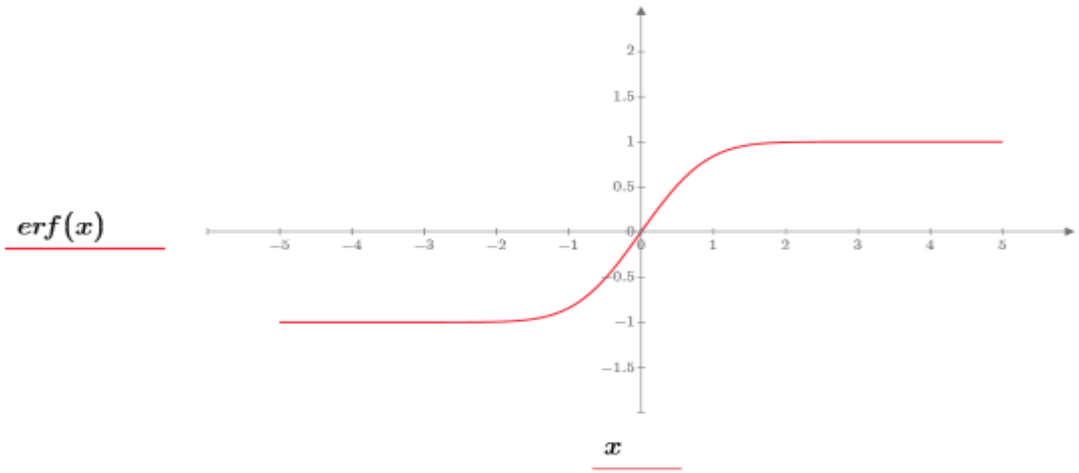

Figure 1.1 (Source: https://support.ptc.com/help/mathcad/r10.0/en/index.html#page/PTC_Mathcad_Help/example_error_functions.html)

2. **Complementary Error Function**: Complementary Error function of x is defined as $\frac{2}{\sqrt{\pi}}\int_x^\infty e^{-u^2}\,du$ and is denoted by erfc(x)

We write

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-u^2}\,du$$

The plot of complementary error function for different values of x are as follow.

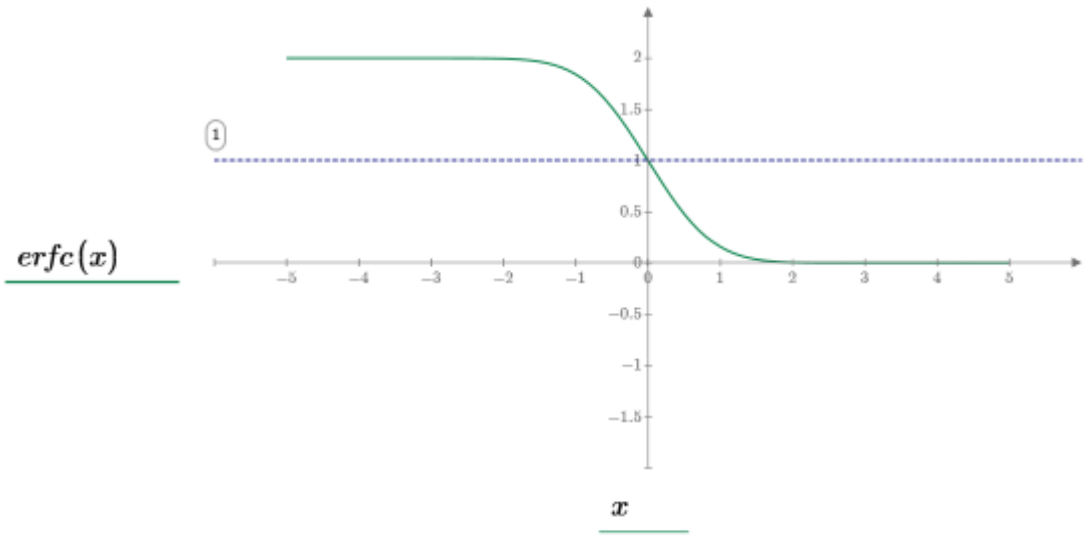

Figure 2.1 (Source:

https://support.ptc.com/help/mathcad/r10.0/en/index.html#page/PTC_Mathcad_Help/example_error_functions.html)

3. Alternate definition of Error Function:

We have $\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du$ if we put $u^2 = t, 2udu = dt$

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^{x^2} e^{-t}\frac{dt}{2\sqrt{t}} = \frac{1}{\sqrt{\pi}}\int_0^{x^2} e^{-t}\,t^{-1/2}dt$$

Therefore

$$\text{erf}(x) = \frac{1}{\sqrt{\pi}}\int_0^{x^2} e^{-t}\,t^{-1/2}dt$$

4. Properties of Error Functions

i. $\text{erf}(\infty) = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-u^2}\,du$

Put $u^2 = y$

$=\frac{2}{\sqrt{\pi}}\int_0^{\infty} e^{-y}\frac{1}{2}y^{-1/2}dy$

$=\frac{1}{\sqrt{\pi}}\int_0^{\infty} e^{-y}\,y^{-1/2}dy$

$=\frac{1}{\sqrt{\pi}}\Gamma\frac{1}{2}$

But $\Gamma\frac{1}{2}=\sqrt{\pi}$

Therefore $\mathbf{erf}(\infty)=\mathbf{1}$

ii. $\text{erf}(0)=\frac{2}{\sqrt{\pi}}\int_0^{0} e^{-u^2}\,du=0$

Therefore $\mathbf{erf}(\mathbf{0})=\mathbf{0}$

iii. $\text{erf(x)}+\text{erfc(x)}=\frac{2}{\sqrt{\pi}}\int_0^{x} e^{-u^2}\,du+\frac{2}{\sqrt{\pi}}\int_x^{\infty} e^{-u^2}\,du$

$=\frac{2}{\sqrt{\pi}}\int_0^{\infty} e^{-u^2}\,du=\text{erf}(\infty)=1$

$\mathbf{erf(x)}+\mathbf{erfc(x)}=\mathbf{1}$

iv. Error function is an odd function

We have $\text{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^{x} e^{-u^2}\,du$

$\text{erf}(-x)=\frac{2}{\sqrt{\pi}}\int_0^{-x} e^{-u^2}\,du$

$put\ u=-y, du=-dy$

And limit also changes to 0 $to\ x$

$\text{erf}(-x)=\frac{2}{\sqrt{\pi}}\int_0^{-x} e^{-y^2}\,(-dy)$

$\text{erf}(-x)=-\frac{2}{\sqrt{\pi}}\int_0^{-x} e^{-y^2}\,dy$

Therefore $\mathbf{erf}(-\boldsymbol{x})=-\mathbf{erf}\ (\boldsymbol{x})$

Thus, error function is an odd function

v. Expression for error function in series

We have, $\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du$

Since $e^{-t} = 1 - t + \frac{t^2}{2!} - \frac{t^3}{3!} + \ldots..$

Therefore

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x [1 - u^2 + \frac{u^4}{2!} - \frac{u^6}{3!} + \cdots.]du$$

$$= \frac{2}{\sqrt{\pi}}\left[u - \frac{u^3}{3} + \frac{u^5}{10} - \frac{u^7}{42} + \cdots..\right]$$

Apply limit from $0\ to\ x$

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}}\left[x - \frac{x^3}{3} + \frac{x^5}{10} - \frac{x^7}{42} + \cdots..\right]$$

This series is uniformly convergent and hence erf(x) is continuous function of x. Values of erf(x) can be calculated by using above series.

vi. Differentiation of Error function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du$$

$$\text{erf}(ax) = \frac{2}{\sqrt{\pi}}\int_0^{ax} e^{-u^2}\,du$$

Using second rule of Differentiation Under Integral Sign (DUIS) , We get

$$\frac{d}{dx}\text{erf}(ax) = \frac{2}{\sqrt{\pi}}\left[\int_0^{ax}\frac{\partial}{\partial x}e^{-u^2}du + \{\frac{d}{dx}(ax)\}e^{-(ax)^2} - \{\frac{d}{dx}(0)\}e^{-0}\right]$$

$$= \frac{2}{\sqrt{\pi}}\left[0 + ae^{-a^2x^2} - 0\right]$$

$$\frac{d}{dx}\text{erf}(ax) = \frac{2ae^{-a^2x^2}}{\sqrt{\pi}}$$

vii. Integration of Error function

$$\int_0^t \text{erf}\,(ax)\,dx = \int_0^t 1.\,\text{erf}\,(ax)\,dx$$

$$Integration\ by\ parts$$

$$= [\text{erf}(ax)\,.\,x] - \int_0^t \frac{d}{dx}\text{erf}(ax)\,.\,xdx$$

$$= t\,\mathrm{erf}(at) - 0 - \int_0^t \frac{2ae^{-a^2x^2}}{\sqrt{\pi}} x dx$$

$$= t\,\mathrm{erf}(at) + \frac{a}{\sqrt{\pi}} \int_0^t e^{-a^2x^2} (-2a^2 x dx)$$

$$= t\,\mathrm{erf}(at) + \frac{1}{a\sqrt{\pi}} \left[e^{-a^2x^2}\right]$$

$$Using\ limit\ from\ 0\ to\ t$$

$$= t.\mathrm{erf}(at) + \frac{1}{a\sqrt{\pi}} \left[e^{-a^2t^2} - 1\right]$$

Therefore $\int_0^t \mathrm{erf}\,(ax)\,dx = t.\mathrm{erf}(at) + \frac{1}{a\sqrt{\pi}} \left[e^{-a^2t^2} - 1\right]$

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COMPREHENSIVE REVIEW ON WAVELET NEURAL NETWORK FOR SOLVING FRACTIONAL DIFFERENTIAL EQUATIONS

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Abstract:

Fractional differential equations have gained great significant attention due to their ability of modelling complex systems with enormous properties. Traditional numerical methods face challenges in optimizing higher order fractional differential equations results to explore unique techniques for precise solutions. This paper provides comprehensive review of the hybrid approach for solving fractional differential equations by the combination of wavelets and Artificial Intelligence algorithms called Wavelet Neural Networks, with applications in several fields such as image processing, cryptographic, and robotics. Further paper discusses about applications of Wavelet Neural Networks in fractional differential equations, foundations, implementation, advantages, and challenges.

Keywords: Fractional Differential Equations, Artificial Intelligence Algorithms, Wavelet Transform, Neural Networks, Wavelet Neural Networks.

Introduction:

Fractional differential equations (FDEs) are powerful tool of mathematics for modelling complex models with long term dependence and memory in various scientific fields (Miller and Ross, 1993). These equations generalize the image of differentiation to non-integer orders by providing powerful framework for describing complex mathematical models by the applicability in diverse fields (Podlubny, 1999) as rheology, dynamical processes in porous structures, signal processing, physics, biology and engineering finance. The general form of FDE is:

$$D^{\alpha} y(t) = f\left(t, y(t)\right),$$

where D^{α} denotes the fractional derivative of α order and $f\left(t, y(t)\right)$ is a function describing the system.

FDEs are difficult to solve, Analytical solution of FDEs is infeasible for higher order systems, needs for innovative numerical methods which are capable of solving FDEs efficiently and accurately (Momani and Odibat, 2007). Traditional methods include Laplace Transform, spectral methods, Adomian decomposition method, homotopy analysis method and fractional linear multi- step method, many traditional methods are designed for solving FDEs but they are not directly implacable due to their fractional properties (Wu *et al.* 2023), leads to explore more techniques for more precise results.

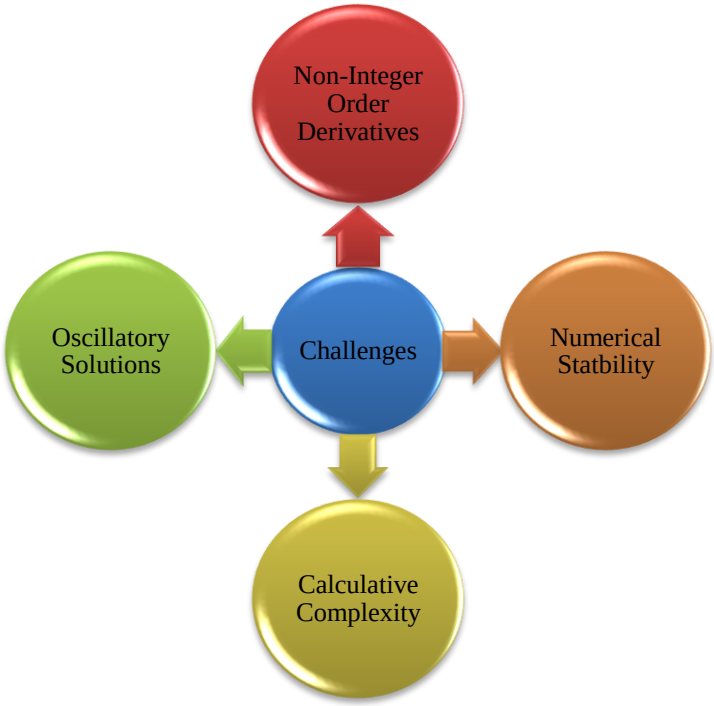

Figure 1: Challenges in Solving FDEs.

The hybrid approach for solving FDEs by the combination of wavelets and Artificial Intelligence (AI) algorithms called Wavelet Neural Networks (WNNs). The WNNs is based on family of wavelets (Alexandridis and Zapranis, 2013). Wavelet transform are mathematical tools used to break down the data into components, localized in both frequency and time by providing the required results. In recent years, the wavelets approach (Rayal and Verma, 2020; Rayal *et al.* 2023; Rayal *et al.* 2024) has become more and more popular in the field of numerical methods. Several wavelet types and approximate functions were used for this (Rayal and Verma, 2020, Rayal and Verma, 2022; Rayal, 2023). Wavelet-based approaches are employed for solving differential equations, particularly non-linear differential equations, providing highly accurate solutions by method of transforming the differential equations into integral equations via integration (Rayal, 2023). The WNNs combines the concept of wavelet analysis with neural networks.

Neural Networks (NNs) are computational models that mimics the way as human brain operates, which is capable of learning complex patterns and functions (Pakdaman *et al.* 2017). WNNs finds various applications in adaptive control systems, environmental data analysis: weather patterns, ocean currents or seismic signals; pattern recognition by presenting data in frequency components, signal processing and image processing (Zhang *et al.* 1995). WNNs consist of multi layers where each layer performs different type of wavelet transform. The structure of proposed algorithm WNNs composed of input layer, wavelet expansion and connected layer and output layer (Wu *et al.* 2023). Neural Networks has excellent performance while dealing with higher order FDEs, involves optimizing the parameters of wavelets function and neural networks layers (Qu *et al.* 2020). This hybrid approach utilizes the strengths of neural networks and wavelet analysis by providing effective solutions. This review examines the methodologies, evolution and applications of WNNs in solving FDEs.

Wavelet Neural Network (WNN)

WNNs integrates the wavelet transforms with NNs which proposes the framework used for solving complex FDEs. We explore the implementation of WNNs on FDEs including processes, advantages and limitations. The algorithm of WNNs for solving FDEs is consist of three-layer components (Li *et al.* 2022): the wavelet transform layer; the neural network layer and the inverse wavelet transform layer. In this first layer, the WNNs uses wavelet function as the basis, transforms the problem where wavelet function acts as building blocks to represents the solution of FDEs. Further, the second NNs layer consist of neurons that uses the transformed data from first layer. NNs layer combines the data which helps in learning the complex patterns needed to approximate the solution. The Output layer or Inverse wavelet transform layer combines the calculated coefficients and wavelet function from second layer, minimizes the error and produces the final approximated solution of inputted FDEs (Rostami and Jafarian, 2018).

The three layers of WNNs works altogether and produces the approximated solution of FDEs by:

- Using input layer of wavelet transform to represent the FDEs.
- Processing the transformed data from input layer by combining the wavelet coefficients.
- Generating the final approximated solution by combining the data transformed from second layer and estimating the errors.

The flexibility of WNNs to tackle the challenges in solving complex FDEs are remarkable. It provides a versatile framework for learning complex patterns by adjusting parameters if inputted FDEs and generating precise solution.

The functioning of layers of WNNs in generating approximated solution operates as follows:

- **Wavelet transform layer (Wu *et al.* 2023)**

Purpose	• Break-downs the input data into multi-resolution components.
Implementation	• The input data is transformed using wavelet transform; captures both high and low frequency detatils in the conerted data.
Process	• The wavelet transform is applied to fuction for obtatining the wavelet coeffecients. The choice of wavelet function affects the accuracy and performance of model.

- **Neural network layer (Li *et al.* 2022)**

Purpose	• Processes the wavelet transformed data to study the complex relation described by FDEs.
Implementation	• Feedforward or deep learning neural network is used to process the wavelet coefficients. Network maps the wavelet coefficents to solution of FDEs.
Training	• NNSs uses pairs of wavelet-transformed inputs known as solution of FDE.

- **Inverse wavelet transform layer (Li *et al.* 2022)**

Purpose	• Reconstructs the final solution of FDE from calculated wavelet coefficients.
Implementation	• The final output of NNs which represents the wavelet coefficient of solution is transformed back using inerse wavelet transform. the approximated solution of FDEs is obtained.

Wavelet Neural Network on FDEs

The hybrid approach of solving FDEs is powerful alternative because of their efficiency, flexibility, adaptability to complex boundary conditions with handling non-linear-higher-order derivatives. Many advanced approaches for finding approximate solution of FDEs are progressed, as elaborated in Table 1.

Table 2: Methods of Solving FDEs using NNs.

S. No.	Method of solution	NNS Architecture	Fractional derivative
1	Admas-Bashforth-Moulton method (Raja *et al.* 2011)	Feed-forward ANNs	Reimann -Liouville derivative
2	Chebyshev wavelet method (Raja *et al.* 2010)	Feed-forward ANNs	Reimann -Liouville and Caputo derivative
3	Collocation method (Yavari, 2019)	Feed-forward ANNs	Caputo derivative
4	Euler method (Pakdaman *et al.* 2017)	ANNs	Atangana-Baleanu in Caputo sense derivative
5	Finite difference method (Sadati *et al.* 2008)	Jacobi orthogonal FANNs	Caputo derivative
6	Laplace transform method (Wu and Zeng, 2016)	Fuzzy FANNs	Caputo derivative
7	Shifted Legendre method (Ghasemi and Nazemi, 2019)	ANNs	Caputo derivative
8	Laplace transform method (Li, 2007)	Backpropagation ANNs	Reimann -Liouville derivative
9	Power series expansion (Petras, 2006)	Cellular FANNs	Grunwald-Letnikov derivative
10	Adomian decomposition method (Hadian-Rasanan *et al.* 2019)	Orthogonal FANNs	Caputo derivative
11	Admas-Bashforth-Moulton method (Yazdizadeh, 2020)	Dynamic FANNs	Caputo derivative

WNNs uses a combination of algorithmic steps to process data by extracting multiple features from provided data in form of FDEs. This process allows WNNs to handle and interpret data structures easily. The given algorithm provides an overview of WNNs for tackling FDEs depending on complexity of specific problem varies to different kind of FDEs. Algorithm used for solving FDEs by using hybrid approach with WNNs is given in Figure 2.

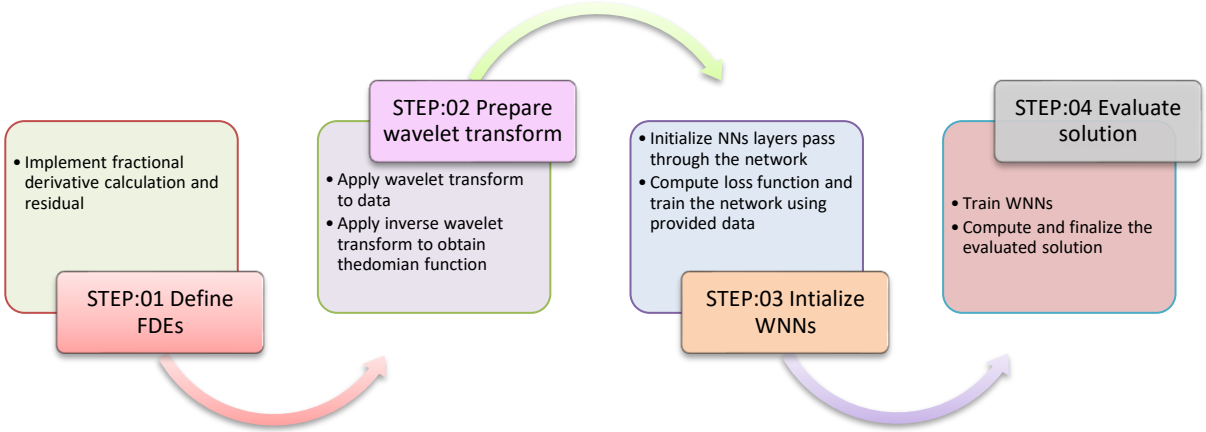

Figure 2: Algorithm used by WNNs.

Advantages and challenges of WNNs

This table highlights the advantages and challenges of WNNs for generating approximate solution of FDEs:

Aspects	Advantages	Challenges
Accuracy	Higher accuracy rate in solving FDEs due to adaptive nature.	Requires extensive training for getting higher accuracy rate.
Flexibility	Flexible in handling various types of FDEs by adjusting wavelet functions.	Choosing suitable wavelet and NNs can be complex.
Error Analysis	Errors can be minimized by suitable selection of NNs and wavelet functions.	Challenging when dealing with higher-order or dimension FDEs.
Computational Efficiency	Efficient due to breaking components of wavelet domain.	Trainings are expensive and time-consuming for large-scale FDEs.
Data Handling	Capable of handling incomplete data effectively by feature extraction.	Requires amount of high-quality data to generalize well.

The future scope that expands capabilities and applications of WNNs on FDEs includes:

- Adaptive methods- learning to handle various types of FDEs and learning new NNs algorithms.
- Handling-large scale Problems- enhancing ability of WNNs to solve non-integer, high-scale FDEs efficiently.
- Real-time Applications- expanding applications to real-time for accurate solutions to FDEs in control systems.
- Enhanced accuracy-advanced NNs and trained techniques for more précised solutions.
- Broader Applications- exploring applications in new fields in relevant areas.

Conclusion:

Wavelet neural networks are emerging powerful tool for solving complex fractional differential equations with several benefits over many traditional methods as they are not directly implacable due to their fractional properties, leads to explore more techniques for more precise results. The applicability and effectiveness of this hybrid approach gives précised results of higher- dimension fractional differential equations. WNNs finds various applications in adaptive control systems, environmental data analysis: weather patterns, ocean currents or seismic signals and exploring applications in many new fields. The hybrid approach by combining wavelet and neural networks shows significant advancement in solving the complex models or fractional differential equations very efficiently. Further, it gives a chance to explore more about the relevant fields in which Wavelet neural network performs effectively.

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STRAIN GAUGES FOR DAMAGE IDENTIFICATION IN ASYMMETRIC SANDWICH COMPOSITES: A COMPARATIVE ANALYSIS OF MATERIALS AND METHODS

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Abstract:

Sandwich composite materials have become increasingly popular in various engineering fields due to their favourable strength-to-weight ratio, structural efficiency, and versatility. However, the inherent complexity of these materials, especially when incorporating natural elements such as cork and stone, introduces challenges in ensuring long-term structural integrity. The use of natural materials in composite structures has gained attention for its environmental benefits, yet their unpredictable mechanical behaviour underscores the need for advanced structural health monitoring (SHM) techniques. Traditional non-destructive testing (NDT) methods, while useful, often require periodic assessments that may not detect damage in real-time, potentially leading to catastrophic failures.

This paper investigates the effectiveness of strain gauges in the real-time detection of damage within asymmetric sandwich composites made from natural materials, specifically cork and stone. The composites, consisting of a core of agglomerated cork with epoxy-reinforced glass fibre layers and a stone exterior, were subjected to destructive bending tests to evaluate their mechanical properties, including tensile, compressive, and flexural moduli. The study compares two configurations: stone facing up and stone facing down, assessing the performance of strain gauges in both scenarios to monitor strain and detect the onset of damage.

The results demonstrate that strain gauges are highly effective in detecting damage within these natural material composites, particularly in identifying critical failure modes such as stone layer crushing and fiber breakage in the epoxy skins. Additionally, the configuration with the stone facing up exhibited superior bending strength, likely due to the stone's higher resistance to compressive forces. This study provides valuable insights

into the mechanical performance and failure behavior of natural material composites, contributing to the growing body of knowledge on SHM for sustainable engineering materials. By defining critical strain thresholds, this research offers a practical pathway for the integration of strain gauges in real-world applications, enabling timely maintenance actions and preventing catastrophic failures.

Keywords: Strain Gauges, Damage Identification, Asymmetric Sandwich Composites

Introduction:

Sandwich composite materials have become increasingly popular in various engineering fields due to their favourable strength-to-weight ratio, structural efficiency, and versatility. However, the inherent complexity of these materials, especially when incorporating natural elements such as cork and stone, introduces challenges in ensuring long-term structural integrity [1]. The use of natural materials in composite structures has gained attention for its environmental benefits, yet their unpredictable mechanical behaviour underscores the need for advanced structural health monitoring (SHM) techniques. Traditional non-destructive testing (NDT) methods, while useful, often require periodic assessments that may not detect damage in real-time, potentially leading to catastrophic failures [2].

Composite materials have transformed modern engineering with their ability to offer high strength, light weight, and adaptability to various structural applications. Among the most widely used are sandwich composites, which consist of a core material sandwiched between two outer layers [3]. These structures are favored for their exceptional stiffness-to-weight ratio, making them ideal for industries such as aerospace, automotive, civil engineering, and marine construction. The design of sandwich composites allows engineers to optimize mechanical performance, but this complexity also brings challenges, particularly in terms of predicting failure modes and ensuring long-term durability [4].

Traditionally, sandwich composites have been composed of synthetic materials such as polymer matrices, carbon fibers, or glass fibers. However, recent shifts toward sustainability and environmental consciousness have led to the exploration of natural materials for use in composite structures. Natural materials like cork and stone offer several advantages, including thermal insulation, soundproofing properties, and a lower environmental impact. Cork, for example, is lightweight, flexible, and has excellent energy absorption characteristics, while stone provides substantial compressive strength and

durability [5]. Yet, integrating these materials into composite structures introduces a level of unpredictability in mechanical behavior due to their heterogeneity and variation in properties.

One of the most critical issues with composite structures, particularly those incorporating natural materials, is the detection and characterization of damage before catastrophic failure occurs [6]. Failure in composite materials can be complex and can manifest in various forms, including fiber breakage, delamination, matrix cracking, and core crushing. Identifying these failures early is essential for maintaining the safety and performance of the structure, particularly in applications where regular inspection is not feasible [7]. While non-destructive testing (NDT) methods such as ultrasonic testing, thermography, and radiography have been employed for damage detection, these techniques often require specialized equipment and periodic inspections. This limitation poses a significant risk, as damage may develop between inspections and remain undetected until it leads to failure.

In contrast, structural health monitoring (SHM) offers a more proactive solution, enabling continuous monitoring of material behavior in real-time [8]. SHM techniques, including the use of embedded sensors such as fiber optic sensors and strain gauges, provide real-time data on strain, deformation, and other critical parameters. Strain gauges, in particular, are simple, reliable, and widely used in engineering for detecting mechanical stress and strain in structures [9]. When applied to composite materials, strain gauges can continuously monitor changes in strain distribution, enabling the early detection of damage, including micro-cracking and fiber-matrix delamination.

Despite the growing body of research on SHM techniques, there is still a significant gap in understanding how these systems perform in sandwich composites made from natural materials. The combination of materials like cork and stone in composite structures has been relatively unexplored in terms of mechanical behavior and failure mechanisms. Furthermore, the impact of sensor integration—such as strain gauges—on the performance of these materials remains under-studied, particularly in asymmetric configurations [10].

This study aims to address these gaps by investigating the mechanical properties and damage detection capabilities of an asymmetric sandwich composite made from a cork core, epoxy-reinforced fiber skins, and a natural stone facing. The primary objectives of the research are to:

1. Characterize the mechanical properties of the composite, including tensile, compressive, and flexural moduli, in both stone-up and stone-down configurations.
2. Evaluate the effectiveness of strain gauges in detecting damage during destructive bending tests, providing real-time monitoring of strain and identifying critical failure modes.
3. Analyze the failure mechanisms of the composite, particularly the differences in behavior between the stone-facing-up and stone-facing-down configurations.
4. Provide insights into the integration of natural materials into composite structures, highlighting the challenges and benefits of using cork and stone in structural applications.

By conducting this research, the study aims to contribute to the advancement of SHM techniques for composite materials, with a particular focus on those made from sustainable, natural resources [11]. The findings are expected to have practical implications for the design and maintenance of composite structures in various engineering fields, offering a pathway to improved safety, durability, and sustainability in future applications. This expanded introduction emphasizes the motivation for the study, the significance of using natural materials in composite structures, and the role of SHM in enhancing safety and durability.

Figure 1: Multi layer composite

Materials and Methods

1. Specimen materials

The specimens were manufactured with a core cork agglomerate (CA) between two glass fibre-reinforced epoxy (GFRE) face sheets complemented by a structural layer of natural stone, as illustrated in Fig. 1. The stone layer, consisting of Creme de F´atima limestone (provided by Filstone), had an average thickness of 7.5 mm, while the CA core (NL20) with an average thickness of 15 mm was provided by Amorim Cork Composites [12]. For the production of the glass fibre face sheets, Epolit RS 7720 epoxy resin from QMC Tecnología Química was used in combination with two distinct types of glass fibres. To

ensure a smoother stiffness transition between the stone and agglomerated cork, the GFRE1 layer employed a stiffer glass fibre, EBXS600, while the GFRE2 layer used UTE 280 T fibre, both sourced from Castro Composites. The specimens were of standard dimensions: 50 mm in width, 23 mm in total thickness, and 300 mm in length [13].

2. Sensors and acquisition system

The sensors used to acquire the strain data were 1-LY16-6/350 strain gauge sensors from Hottinger Baldwin Messtechnik (HBM). Two strain gauges were placed on opposite sides (one at stone layer and the other one at the GFRE2 layer) of the specimens for the purpose of conducting mechanical characterization of this composite [14]. The location of both strain gauges is presented in Fig. 2, where L corresponds to the specimen's length (300 mm) while W represents the width of the specimen. SG_c and SG_t correspond to the strain gauge found at the compressive and tensile sides, respectively. To obtain the strain measurements from the strain gauge sensors, a NI-9237 module provided by National Instruments (NI) was utilized [15]. A data acquisition rate of 1613 Hz was employed for the strain gauge measurements. The sensors were connected in a Wheatstone bridge configuration, more specifically a quarter bridge with a dummy strain gauge (configuration type II). The NI-9237 module was also connected to a computer with LabView software.

3. Destructive bending tests without sensors

The four-point bending test was used, with loading points spaced one-third of the supporting span apart, in accordance with the procedures outlined in the ASTM C393/C393M standard. An Instron 5566 universal testing machine with a 10 kN load cell was used to perform the bending tests [16]. According to M. Garcia's guidelines, the testing process was conducted with a top roller velocity set at 3 mm/min and a preload of roughly 10 N applied consistently prior to each test [17]. The testing apparatus was linked to Bluehill Universal software, enabling the recording of load, top roller displacement, and time data at a frequency of 50 Hz. The samples were tested with both sides of the stone facing up [18].

4. Mechanical characterization

To ascertain the various mechanical characteristics of this substance and identify the neutral line, the process delineated by Mujika *et al.* was done [19]. At the surface of the GFRE2 layer and the surface of the stone layer, respectively, two strain gauges were affixed to the specimens. The same setup as previously mentioned was used for the four-point bending testing. In this instance, though, the specimens were tested with their backs to the

stone, and a maximum load of 515 N was applied [20]. This maximum load is equal to 25% of the average maximum load that the composite could sustain when subjected to the identical configuration (stone facing up) in destructive bending tests [21].

5. Destructive bending tests with sensors

The process described in section 2.3 was repeated after the instrumented specimens were mechanically characterized. In this case, however, strain data was constantly recorded until the material failed from both strain gauges inside the specimens [22]. As mentioned earlier, the purpose of this method was to evaluate the sensitivity of strain gauges in identifying deterioration in the composite [23].

Results:

1. Destructive bending without sensors

The composite was tested until failure in both facing up and stone facing down configurations, as previously described. The relevant stress vs. displacement curves are shown in Figs. 4a and 4b, respectively. When testing in the stone facing up configuration, it is clear from comparing Figs. 4a and 4b that this composite had a higher bending strength, which can be attributable to the stone's stronger resistance to compressive stress [21]. Additionally, the specimens failed at a lower displacement level (about 5 mm) in the stone facing down configuration than at the same value (about 15 mm) in the stone facing up configuration. This implies that when tested in the stone face up arrangement, the material shows better ductility. Table 1 shows the average values for both configurations and the corresponding standard deviations for the bending strength obtained for the various tested specimens in the stone facing down and up configurations [22].

When the material was evaluated in the stone facing up configuration, a larger variability was discovered, according to the data in Table 1. An examination of the primary mode of failure for every configuration can offer valuable perspectives for comprehending the observed fluctuation. The catastrophic collapse at the stone layer happened in the stone facing up configuration (Fig. 5a), whereas in the stone facing down, the GFRE2 layer experienced similar failure (Fig. 5b). This variation in unpredictability can be linked to the inherent characteristics of stone, which is more variable by nature [23], in contrast to GFRE2, which is made of two artificial materials. When the actual average bending strength values for the two configurations are compared, though, the variability in the stone facing down configuration (roughly 24% of the average bending strength) is more noticeable than in the stone facing up configuration (roughly 8% of the corresponding average bending strength value). Nevertheless, both variability values were less than those observed in the

actual natural stone [24]. This is important because it helps design engineers choose appropriate safety parameters for the material's application. Due to the higher bending strength values obtained, the stone face up arrangement was the only one analysed in the next steps [25].

2. Mechanical characterization

Before presenting the determined mechanical properties, it is important to evaluate the repeatability and reproducibility of the data obtained using strain gauges across multiple repetitions [26]. Tables 2 and 3 list the strain data obtained when applying the maximum load in this scenario, at the stone and GFRE2 outer surface layers, respectively. As previously stated, two strain gauges were placed on opposite sides of the composite (the outer surface of stone and GFRE2 layers). The specimens were tested using the same previously described methodology [27].

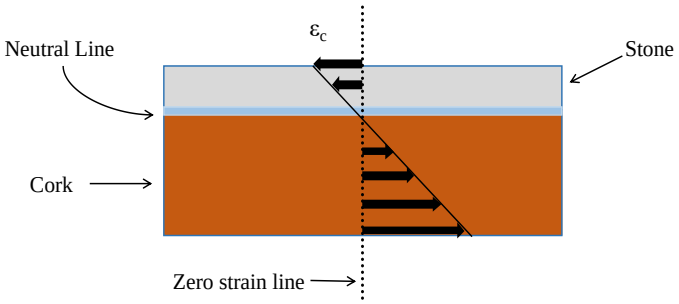
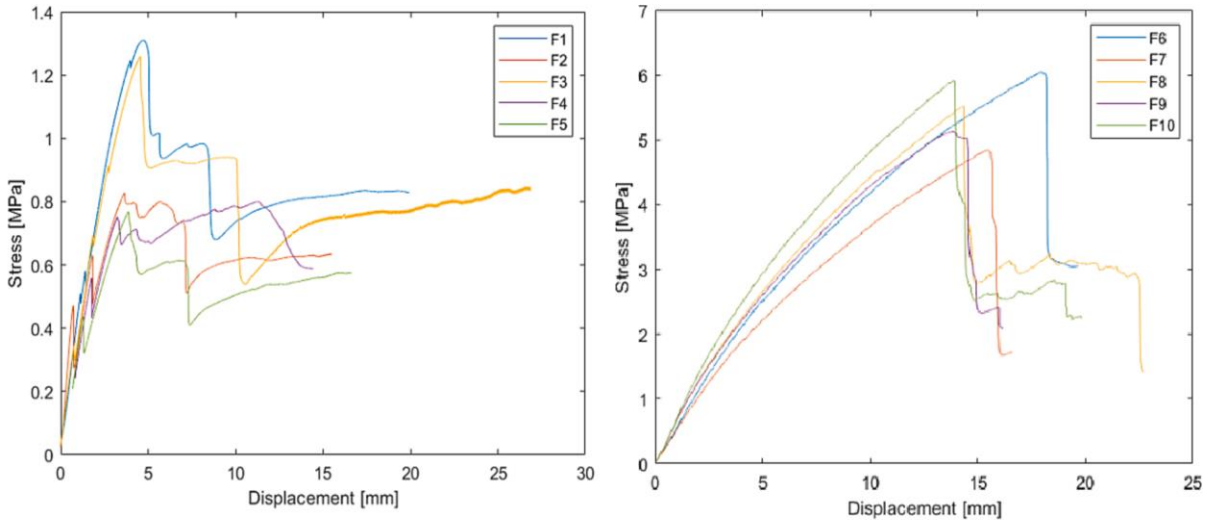


Figure 3: Schematic of the Strain distribution throughout the thickness of the composite



(a) (b)

Figure 4: Stress vs displacement curves for:
a) stone facing down configuration; b) stone facing up configuration

Table 1: Bending Strength found for both stone facing down and up configuration

Stone facing down configuration		**Stone facing up configuration**	
Specimen	Bending Strength [MPa]	Specimen	Bending Strength [MPa]
F1	1.31	F6	6.05
F2	0.83	F7	4.85
F3	1.26	F8	5.52
F4	0.8	F9	5.13
F5	0.77	F10	5.92
Average	0.99 ± 0.24	Average	5.49 ± 0.46

(a) **(b)**

Fig. 5. Predominant failure modes:

a) Stone facing up configuration; b) Stone facing down configuration.

Table 2 makes it clear that during the five repetitions within the same specimens, the strain data recorded at the stone surface stayed constant. The low standard deviation values found for every specimen further support this great degree of uniformity.

Table 2: Strain values measured at stone surface layer for the different specimens (absolute value)

Specimen	ε_{C1}	ε_{C2}	ε_{C3}	ε_{C4}	ε_{C5}	$\overline{\varepsilon_C}$	**SD**	**CV (%)**
FS1	6.50E-04	6.50E-04	6.50E-04	6.80E-04	6.60E-04	6.60E-04	1.30E-05	2
FS2	5.90E-04	5.90E-04	5.80E-04	6.00E-04	5.80E-04	5.90E-04	6.70E-06	1.1
FS3	5.40E-04	5.60E-04	5.60E-04	5.60E-04	5.60E-04	5.60E-04	9.00E-06	1.6
FS4	7.10E-04	7.20E-04	7.10E-04	7.00E-04	7.20E-04	7.10E-04	7.40E-06	1
FS5	5.40E-04	6.20E-04	6.20E-04	6.10E-04	6.10E-04	6.00E-04	3.10E-05	5.2

Table 3 revealed a similar pattern, confirming the consistency and dependability of the strain data collected during the experimental testing [28]. The failure modes that were found provide credence to the concept that the strain is continuous throughout the thickness of the specimens. If this weren't the case, delamination would be expected and apparent relative movement would probably come from a poor adhesion process [29]. Therefore, the neutral line location for each of the tested specimens was inferred using the data in Tables 2 and 3.

Table 3: Strain values measured at GFRE2 surface layer for the different specimens

Specimen	ε_{T1}	ε_{T2}	ε_{T3}	ε_{T4}	ε_{T5}	$\overline{\varepsilon_T}$	SD	CV (%)
FS1	2.60E-03	2.70E-03	2.70E-03	2.70E-03	2.70E-03	2.70E-03	3.40E-05	1.3
FS2	1.90E-03	1.90E-03	1.90E-03	1.90E-03	1.90E-03	1.90E-03	7.50E-06	0.4
FS3	1.90E-03	1.90E-03	1.90E-03	1.90E-03	1.90E-03	1.90E-03	1.10E-05	0.6
FS4	2.70E-03	2.80E-03	2.80E-03	2.80E-03	2.80E-03	2.80E-03	2.60E-05	0.9
FS5	2.10E-03	2.00E-03	2.10E-03	2.00E-03	2.10E-03	2.10E-03	1.10E-05	0.5

Table 4 results demonstrated that, for the same specimen, the neutral line placements obtained were consistent across all five tests, with a standard deviation of less than 0.10 mm.

Table 4: Neutral line location (in mm) using only strain data

Specimen	N_{L1}	N_{L2}	N_{L3}	N_{L4}	N_{L5}	$\overline{NL}$	SD	CV(%)
FS1	4.39	4.4	4.34	4.51	4.41	4.41	0.05	1.13
FS2	5.46	5.14	5.29	5.5	5.34	5.35	0.13	2.43
FS3	5.18	5.03	5.3	5.44	5.18	5.23	0.14	2.68
FS4	4.72	4.77	4.66	4.6	4.66	4.68	0.06	1.28
FS5	5.34	5.18	5.3	5.17	5.2	5.24	0.07	1.34

An anomaly was discovered in the FS5 specimen, which showed a 4.22% coefficient of variation with a standard deviation of 0.22 mm Nevertheless, following the removal of

the outlier value (NL = 4.78 mm). There was a standard deviation of less than 0.05 mm and an average neutral line placement of 5.31 mm. They varied from 4.55 to 5.34 mm when taking the average values into account. The observed variation can be explained by the variability of the materials employed in the production of the two skins, including stone and agglomerated cork. Starting at the top of the stone layer, the neutral line is measured. The neutral line of this composite was found inside the stone layer, based on the average thickness of the stone layer (7.5 mm). This could seem problematic at first because it indicates that there may be tensile stresses in some part of the stone layer, and stone is known to have a higher resistance to compression loading. But considering the primary mode of failure in this instance, which was stone crushing, it suggests that the stone was resilient enough to withstand the degree of tensile stresses that came from the bending tests. Alternatively, the neutral line location can be found by adopting the methodology proposed by Mujika *et al.* [30], and the results are displayed in Table 5. Over the course of the five repeats, a reduced dispersion (below 0.15 mm) within the same specimens is consistently obtained by applying the Mujika *et al.* [30] methodology for identifying the neutral line location. The low coefficient of variation levels—all under 3%—provide evidence for this. It is feasible to see a dispersion level (between 4.41 mm and 5.35 mm) that is comparable to the previous one (between 4.55 mm and 5.35 mm) when comparing the average location of the neutral line. The previously listed variables can be ascribed to this variation. The average values for the neutral line location determined by both techniques are shown in Table 6, along with the corresponding percentual difference (PD).

The modest percentual difference figures suggest that the neutral line locations produced by the two approaches are comparable. The methods suggested by Mujika *et al.* [30] can also be used to calculate the composite's tensile, compressive, and flexural moduli. The various modulus values obtained for various specimens and repetitions are listed in Tables 7–9. The constancy of various moduli within the same specimen across five repetitions is highlighted in the study shown in Tables 7–9. The low standard deviation values in comparison to the real moduli values make this clear. With a maximum value of 2%, the low coefficient of variation figures further confirm the consistency of the findings.

However, when comparing the average moduli values observed across different specimens, a significant degree of dispersion might be detected. Once more, the hand lay-up approach utilized to manufacture the two skins and the heterogeneity of the stone and agglomerate are the reasons for this variety. In general, the material displayed greater

compressive modulus values compared to the other two moduli. This is explained by the fact that these characteristics were established in the stone facing up configuration, where the stone was mostly compressed but also exhibits more stiffness than the other components of this composite.

Table 5: Neutral line location (in mm) using Mujika *et al.* methodology

Specimen	NL_1	NL_2	NL_3	NL_4	NL_5	$\overline{NL}$	SD	CV(%)
FS1	4.39	4.4	4.34	4.51	4.41	4.41	0.05	1.13
FS2	5.46	5.14	5.29	5.5	5.34	5.35	0.13	2.43
FS3	5.18	5.03	5.3	5.44	5.18	5.23	0.14	2.68
FS4	4.72	4.77	4.66	4.6	4.66	4.68	0.06	1.28
FS5	5.34	5.18	5.3	5.17	5.2	5.24	0.07	1.34

Table 6: Comparison between the average neutral line location obtained from both methods and correspondent percentual difference (PD)

Specimen	NL_{2ext}[mm]	NL_{sd}[mm]	PD_{2ext}[%]
FS1	4.41	4.55	3.08
FS2	5.35	5.34	0.19
FS3	5.23	5.33	1.88
FS4	4.68	4.75	1.47
FS5	5.24	5.21	0.58
Average	4.98	5.04	1.19

Table 7 Tensile modulus (in MPa).

Specimen	E_{t1}	E_{t2}	E_{t3}	E_{t4}	E_{t5}	$\overline{E_t}$	SD	CV(%)
FS1	803.2	784.7	767.1	809	800.3	792.8	15.2	1.9
FS2	1248.4	1190.6	1211.7	1222.9	1207.4	1216.2	19.1	1.6
FS3	1197.7	1145.8	1169.7	1213.7	1166.8	1177.1	23	2
FS4	804.8	804.4	779	769.6	771.4	785.8	15.6	2
FS5	1141.2	1125.3	1094.4	1108.3	1110	1115.8	16	1.4

Table 8: Compressive modulus (in MPa).

Specimen	E_{c1}	E_{c2}	E_{c3}	E_{c4}	E_{c5}	$\overline{E_c}$	SD	CV(%)
FS1	3428.5	3348.9	3325.8	3348.2	3400.7	3370.4	38.1	1.1
FS2	3963.2	4086.8	4015.8	3943.2	3943.2	3990.5	83.4	2
FS3	4166.8	4162.1	3979.3	3982.3	4083.1	4074.8	82.2	2
FS4	3140.8	3091	3064.8	3058.4	3058.4	3082.7	38.1	1.2
FS5	3836.3	3877	3661	3830.9	3810.7	3792.7	72.5	1.9

Table 9: Flexural modulus (in MPa)

Specimen	E_{f1}	E_{f2}	E_{f3}	E_{f4}	E_{f5}	$\overline{E_f}$	SD	CV(%)
FS1	2190	2060.2	2025.9	2099.1	2097.7	2078.4	31	1.5
FS2	2857.7	2856	2818	2830.7	2850.4	2850.4	24.3	0.9
FS3	2879.6	2811.1	2794.5	2851.8	2833.1	2833.4	29.4	1
FS4	2879.6	2817.7	1975.9	1967.7	1967.7	2679.7	43.8	1.6
FS5	2694.3	2703.8	2594.6	2666.9	2662.7	2664.5	38.3	1.4

3. Destructive analysis

Lastly, the specimens that had been instrumented with strain gauges—which had been used to determine the various moduli previously presented—were tested until they failed. Throughout the entire test, the strain data collected from both strain gauges was continuously recorded. Figure 6 shows the strain levels that were obtained during the bending test for two different specimens, as well as the corresponding instances of catastrophic failure (shown by the red line at Fig. 6a). Figure 6b shows, using a Digital Image Correlation system (VIC 2D), the strain distribution in the horizontal direction throughout the composite at the instant of catastrophic failure.

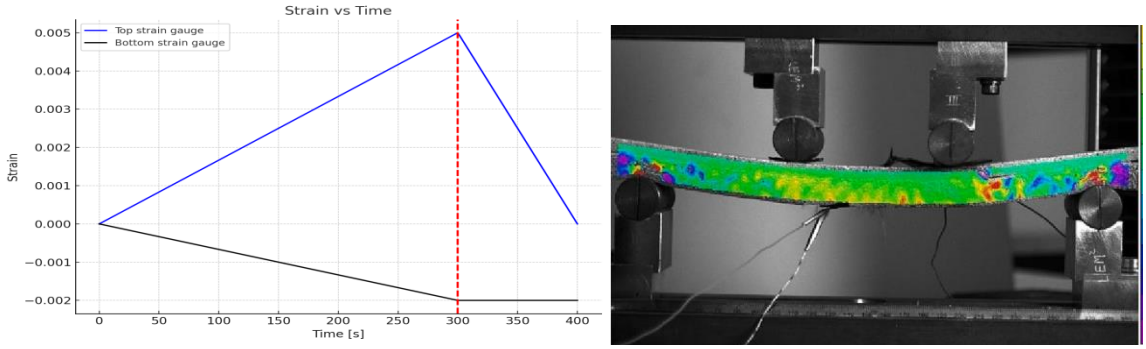
The bottom strain gauge, which was positioned at the GFRE2 layer, as shown in Fig. 6a, recorded greater strain values, indicating that a larger portion of the composite was subjected to tensile stresses. This observation is consistent with the location of the neutral line that was previously determined and with the schematic shown in Figure 3.There are two distinct phases to the strain data from the bottom layer (Fig. 6a): a mainly linear phase in the first 50 seconds of the test, and a following stage that ends in catastrophic failure. The composite was in the elastic domain, as shown by the linear phase. The composite

entered the plastic domain at about the 50-second mark and continued until it reached the catastrophic failure layer [31].

Figure 6a demonstrated that both strain gauges simultaneously detected the catastrophic failure of both specimens (as shown in Figure 6b), even when the failure happened at the layer where the top strain gauge was positioned. These two examples show how well strain gauges work to find this kind of catastrophic damage in this material. The observed mechanism of failure, namely in the stone face up configuration, was caused by the catastrophic fracture of natural stone, a brittle material. Because these materials often break suddenly, this feature makes damage assessments difficult to implement. Acquiring knowledge in advance of failure is essential for prompt maintenance interventions. By using the data from strain gauges, a strain threshold can be set, preventing catastrophic collapse and enabling continuous structural integrity monitoring.

Preventive actions

Tests were conducted on the composite material in both facing down and stone facing up combinations. The substance showed more bending strength when arranged with the stone face up. To fully utilize the potential of this material, it is therefore advised to orient the stone layer in the direction of loading in an application situation. Furthermore, the strain levels that the material encountered throughout the destructive bending tests using strain gauges were noted down to the point of failure. To determine a safe strain threshold for this material's use, it is advised to use this data in conjunction with the integration of strain gauges in practical applications.



(a) **(b)**

Fig. 6. (a) strain evolution for both strain gauges throughout the bending test; (b) strain distribution (in the horizontal direction) at the fracture instant

Conclusion:

In this study, the mechanical characterisation of an asymmetric sandwich composite material with a stone layer on top and an agglomerate cork core sandwiched between two glass fiber reinforced epoxy skins was carried out. Two series of bending tests were run to assess the material's behavior.

Stone facing up and down were the two orientations in which the composite material was tested until it fractured in the first series of testing. This made it possible to calculate the bending strength and identify the main failure modes in both layouts. When tested in the stone facing up configuration, the composite showed stronger bending strength, mainly because stone has a higher resistance to compression, according to the data. Stone crushing was the main failure mode in the stone facing up configuration, whereas fiber breaking within the GFRE2 layer was the main failure mode in the stone facing down configuration. Future applications of this substance should consider this information. To fully utilize the potential of this material, it is therefore advised to orient the stone layer in the direction of loading in an application setting. Moreover, the variability found for both bending strength values was lower than that found for natural stones alone, which is significant in the material's application and helps design engineers determine appropriate safety factors.

In addition to finding the neutral line within the composite, the second set of experiments sought to determine the tensile, compressive, and flexural moduli. The identical specimen's results were consistent across all five repeats, guaranteeing the reproducibility of the outcomes. Nonetheless, the natural variability of stone and agglomerate cork, the hand layup method used to create both skins, and the thickness of the stone layer can all be blamed for differences between various specimens. The results showed that the neutral line for every examined specimen was found inside the stone layer (average position 5 mm; average stone layer 7.5 mm). This suggests that some of the stone layer was subjected to tensile loading during the bending tests. Even though stone resists compression more than tensile loads, this did not cause an issue because stone crushing is the most common form of failure. Numerical models of this composite can be developed or improved using the various experimental data, potentially enabling the material to be accurately simulated in a given application.

Lastly, specimens equipped with strain gauges underwent one more bending test. Throughout the experiment, strain data from both sensors was continuously recorded, and

the specimens were tested until they failed. The catastrophic damage was detectable by both strain gauges. It is best to obtain information before a problem occurs so that maintenance may be carried out on schedule. In addition, the strain gauge data can be used to establish a critical strain threshold, which would prevent the composite from failing catastrophically and allow for continuous structural integrity monitoring.

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INNOVATIVE APPROACHES IN TECHNOLOGY

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Abstract:

Technological advancements are transforming industries by introducing innovative approaches that optimize operations, enhance security, and provide greater data insights. This paper focuses on five key emerging technologies—Artificial Intelligence (AI), Big Data, Cloud Computing, Blockchain, and the Internet of Things (IoT)—and their role in revolutionizing industries. We examine current applications, challenges, and future prospects, with reference to recent academic and industry research. This paper delves into the innovative approaches within these technologies, examining their current applications, the challenges they present, and their future potential for further transforming global industries. Overall, these technologies promise to unlock new efficiencies and opportunities, positioning organizations for success in an increasingly competitive landscape.

Keywords: Innovation, Artificial Intelligence, Big Data, Cloud Computing, Blockchain, Internet of Things (IoT)

Introduction:

Innovation in technology is driving significant changes across various industries, with breakthroughs in Artificial Intelligence (AI), Big Data, Cloud Computing, Blockchain, and the Internet of Things (IoT) serving as pivotal forces in this transformation. These advancements are reshaping the operational landscape by optimizing processes, enhancing decision-making capabilities, and fostering the development of new business models.

Artificial Intelligence has become central to many industries by automating routine tasks, enabling predictive analytics, and optimizing decision-making processes. From healthcare to finance, AI applications are reshaping industries by making them more data-driven and efficient (Topol, 2019; Kou *et al.,* 2021). Similarly, Big Data has become critical in sectors like healthcare, retail, and finance by enabling organizations to leverage large, unstructured datasets to make informed decisions (Raghupathi & Raghupathi, 2014; McAfee & Brynjolfsson, 2012).

Cloud Computing has also revolutionized how businesses manage their IT infrastructure by offering scalable, on-demand computing power, reducing the need for expensive hardware (Armbrust *et al.,* 2010). In parallel, Blockchain technology is transforming industries like finance, supply chain management, and healthcare by providing secure, decentralized transaction platforms (Nakamoto, 2008; Saberi *et al.,* 2019). Lastly, IoT is enabling real-time data exchange and automation in smart cities, industrial automation, and healthcare (Gubbi *et al.,* 2013; Boyes *et al.,* 2018).

These technological advancements, while offering significant benefits, also present challenges such as security risks, ethical concerns, and regulatory issues. This paper examines the current landscape of these technologies, identifies the hurdles to their adoption, and explores the potential they hold for future innovation.

Research objectives

The primary objective of this paper is to:

1. Analyze the current state of technological innovation.
2. Identify applications and challenges in key sectors.
3. Highlight future directions and opportunities for research and development.

Emerging technologies

1. Artificial Intelligence (AI)

Artificial Intelligence (AI) refers to the simulation of human intelligence in machines programmed to think and learn. By utilizing algorithms and large datasets, AI enables systems to perform tasks that typically require human cognition, such as problem-solving, pattern recognition, and decision-making. Key applications of AI include natural language processing, computer vision, robotics, and predictive analytics. As AI continues to advance, it holds the potential to transform various sectors, enhancing efficiency, driving innovation, and enabling more informed decision-making. However, it also raises ethical considerations and challenges related to privacy, bias, and employment.

Key innovations

- Deep Learning: Deep learning, especially through architectures like Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), has significantly enhanced AI's capabilities in image and speech recognition. The introduction of Generative Adversarial Networks (GANs) has further expanded AI's ability to generate synthetic data (LeCun *et al.,* 2015; Goodfellow *et al.,* 2014).

- Natural Language Processing (NLP): Innovations in NLP, particularly through transformer models like BERT and GPT, have vastly improved AI's understanding of human language. These advancements enable more sophisticated applications such as chatbots and language translation (Vaswani *et al.,* 2017; Devlin *et al.,* 2018).
- Reinforcement Learning (RL): RL has achieved notable successes in game-playing AI, such as AlphaGo and AlphaZero, demonstrating superhuman performance by learning through self-play. Its applications also extend to autonomous systems like self-driving cars (Silver *et al.,* 2016; Silver *et al.,* 2018).
- Edge AI and Federated Learning: Edge AI allows for real-time data processing on devices, enhancing privacy and reducing latency. Federated learning enables AI models to learn from decentralized data without compromising sensitive information (Shi *et al.,* 2016; McMahan *et al.,* 2017).
- Explainable AI (XAI): With increasing complexity in AI systems, XAI focuses on transparency and interpretability. Techniques like LIME and SHAP provide human-understandable explanations for model predictions, crucial in high-stakes fields like healthcare and finance (Ribeiro *et al.,* 2016; Lundberg & Lee, 2017).

Applications of AI innovations

- Healthcare: AI innovations enhance diagnostics, predict patient outcomes, and accelerate drug discovery, allowing for personalized medicine (Topol, 2019; Chen *et al.,* 2018).
- Autonomous Systems: AI technologies drive advancements in autonomous vehicles, making them safer and more reliable for real-world deployment (Kendall *et al.,* 2019).
- Finance: The financial sector utilizes AI for risk management, fraud detection, and algorithmic trading, improving decision-making processes (Kou *et al.,* 2021).
- Creative Industries: AI contributes to content generation across various artistic fields, prompting discussions about the intersection of human and machine creativity (Elgammal *et al.,* 2017).

Challenges and future directions

Despite the promise of AI innovations, challenges remain, particularly concerning ethical implications, data privacy, and AI-human collaboration. Issues such as bias and fairness in AI decision-making require ongoing research and innovative solutions to mitigate potential inequalities (Mehrabi *et al.,* 2021). Furthermore, developing efficient

methods for human-AI collaboration is essential for future advancements (Gunning *et al.,* 2019).

2. Big Data

Big Data refers to the vast and complex volumes of structured and unstructured data generated from various sources, including social media, sensors, transactions, and more. Characterized by the "three Vs"—Volume, Velocity, and Variety—Big Data requires advanced analytics and processing tools to extract meaningful insights. Organizations leverage Big Data to improve decision-making, enhance customer experiences, optimize operations, and drive innovation. However, challenges such as data privacy, security, and the need for skilled personnel must be addressed to fully realize its potential in transforming industries. Big Data encompasses vast amounts of data generated in the digital era, driving organizational transformation in data collection, processing, and analysis.

Key innovations in big data

- Data Storage and Management: Innovations like Hadoop and NoSQL databases (e.g., MongoDB, Cassandra) have revolutionized data management by providing scalable and flexible solutions for handling large datasets (García-Molina *et al.,* 2016). Cloud storage has further enhanced data accessibility while reducing costs (Böhm *et al.,* 2014).
- Data Processing Frameworks: Apache Spark enables real-time data processing and analytics, significantly speeding up analysis through in-memory processing (Zaharia *et al.,* 2016).
- Machine Learning and Artificial Intelligence: The integration of machine learning with Big Data technologies facilitates predictive analytics and data-driven decision-making across various sectors (García *et al.,* 2020). Deep learning algorithms are particularly effective for analyzing unstructured data (Khan *et al.,* 2021).
- Data Visualization: Advanced tools like Tableau and Power BI improve stakeholders' ability to interpret complex datasets, enhancing decision-making processes (Kirk, 2016).
- Real-Time Analytics: Technologies such as Apache Kafka enable streaming data processing, crucial for industries like finance that require immediate insights (Dummit *et al.,* 2018).

Applications of big data innovations

- Healthcare: Predictive analytics and personalized treatment plans have emerged from Big Data innovations, improving patient outcomes (Topol, 2019).
- Finance: Innovations support fraud detection, risk management, and algorithmic trading through advanced data analytics (Kou *et al.,* 2021).
- Retail and Marketing: Big Data analytics enhances understanding of customer behavior and improves targeted marketing (Matz *et al.,* 2017).
- Manufacturing: Innovations optimize supply chain management and predictive maintenance, reducing operational costs (Zhao *et al.,* 2019).

Challenges and future directions

- Data Privacy and Security: Ensuring compliance with regulations like GDPR remains a significant challenge, necessitating innovations in data anonymization and encryption (Martin *et al.,* 2019).
- Skill Gap: A shortage of skilled professionals in Big Data analytics emphasizes the need for enhanced education and training (Marr, 2018).
- Future Trends: The rise of automated and self-service analytics will empower non-technical users to engage with data independently. Additionally, edge computing innovations are expected to improve real-time data processing capabilities (Chen *et al.,* 2021).

3. Cloud computing

Cloud computing has fundamentally transformed the management and deployment of IT resources, offering scalable, flexible, and cost-effective solutions for various industries. This summary highlights the significant innovations in cloud computing, their applications, challenges, and potential future directions. Cloud computing is a technology that enables on-demand access to computing resources—such as servers, storage, databases, networking, software, and analytics—over the Internet. It allows organizations to use these resources without the need for physical infrastructure, promoting flexibility, scalability, and cost-efficiency. Cloud services are typically categorized into three main models: Infrastructure as a Service (IaaS), Platform as a Service (PaaS), and Software as a Service (SaaS). While cloud computing offers numerous benefits, including easier collaboration and remote access, challenges such as data security, compliance, and vendor lock-in must be managed to ensure effective implementation.

Key innovations:

- Service Models: The development of diverse service models such as IaaS, PaaS, SaaS , and newer models like FaaS and CaaS allows organizations to select tailored solutions based on their needs (Mell & Grance, 2011; Eisenberg *et al.,* 2020).
- Deployment Models: Innovations in hybrid and multi-cloud deployment models enhance flexibility and efficiency, enabling organizations to utilize multiple cloud providers and on-premises infrastructure (Zhang *et al.,* 2010).
- Serverless Computing: This paradigm allows developers to run applications without managing servers, offering automatic scaling and a pay-as-you-go pricing model (Baldini *et al.,* 2017).
- Edge Computing: Integrating edge computing with cloud technology reduces latency by processing data closer to its source, benefiting IoT and real-time analytics applications (Shi *et al.,* 2016).
- AI and ML Integration: Cloud platforms are increasingly incorporating AI and ML capabilities, facilitating the rapid development of intelligent applications (Zhang *et al.,* 2018).

Applications:

- Healthcare: Secure patient data storage and sharing, telemedicine, and big data analytics for personalized treatment (Hasselgren *et al.,* 2019).
- Finance: Enhanced data management and regulatory compliance, supporting real-time analytics for better decision-making (Garg *et al.,* 2018).
- Education: Accessible cloud-based learning platforms enabling personalized and scalable educational resources (Kerr, 2018).
- E-commerce: Improved scalability during peak seasons and enhanced inventory management through advanced analytics (Choudhury *et al.,* 2019).

Challenges:

- Data Security and Privacy: Compliance with regulations like GDPR necessitates ongoing innovations in data protection (Zissis & Lekkas, 2012).
- Vendor Lock-in: Dependence on a single cloud provider can hinder migration to other platforms, although multi-cloud strategies may alleviate this risk (Marston *et al.,* 2011).
- Skill Shortages: The fast-paced evolution of cloud technologies demands continuous investment in workforce training (Marr, 2018).

Future directions:

Emerging trends include the adoption of quantum computing, increased automation through AI, and enhanced interoperability among cloud services, promising further advancements in cloud capabilities (Saha *et al.,* 2020).

4. Blockchain

Blockchain technology has rapidly evolved beyond its initial application in cryptocurrencies, bringing significant innovations across various sectors. This summary encapsulates key advancements, applications, challenges, and future directions in blockchain technology. Blockchain is a decentralized, distributed ledger technology that records transactions across multiple computers in a way that ensures security, transparency, and immutability. Each transaction is grouped into blocks and linked in chronological order, forming a chain that is difficult to alter retroactively. Originally developed as the underlying technology for cryptocurrencies like Bitcoin, blockchain has since found applications in various sectors, including finance, supply chain management, healthcare, and more. Key features of blockchain include its resistance to tampering, enhanced security through cryptographic techniques, and the ability to facilitate smart contracts—self-executing agreements coded directly into the blockchain. While blockchain presents significant opportunities for innovation, challenges such as scalability, energy consumption, and regulatory concerns remain.

Key innovations

- Decentralization and Distributed Ledger Technology (DLT): Blockchain operates on a decentralized architecture, allowing all participants to access the same data, which enhances transparency and trust (Narayanan *et al.,* 2016).
- Smart Contracts: Self-executing contracts with code-based terms automate enforcement, reducing the need for intermediaries (Christidis & Devetsikiotis, 2016). Platforms like Ethereum facilitate decentralized applications (dApps).
- Interoperability Solutions: Innovations such as cross-chain communication protocols (e.g., Polkadot, Cosmos) enable different blockchains to interact, enhancing usability across applications (Zhang *et al.,* 2020).
- Scalability Solutions: Layer-2 solutions and sharding techniques address scalability issues by increasing transaction throughput and reducing latency (Buterin, 2018).

- Privacy Enhancements: Technologies like zk-SNARKs allow for private transactions while maintaining security and verification, enabling confidential transactions on public blockchains (Zcash, 2016).

Applications

- Finance and Banking: Blockchain enables faster, cheaper cross-border payments and the rise of cryptocurrencies as alternative currencies (Catalini & Gans, 2016).
- Supply Chain Management: Provides immutable records of product provenance, enhancing transparency and accountability in supply chains (Kamble *et al.,* 2019).
- Healthcare: Facilitates secure sharing of patient records, drug traceability, and improved clinical trial transparency (Azaria *et al.,* 2016).
- Voting Systems: Increases the security and transparency of voting processes, helping to reduce fraud (Dunleavy *et al.,* 2019).
- Real Estate: Simplifies property transfers and enhances ownership transparency through smart contracts (Koshy *et al.,* 2019).

Challenges and future directions

- Regulatory Uncertainty: The evolving regulatory landscape creates uncertainty for businesses and investors (Zohar, 2015).
- Energy Consumption: High energy usage in proof-of-work systems necessitates innovations in consensus algorithms, like proof-of-stake (Buterin, 2017).
- Scalability: Continued advancements in scalability solutions are vital for widespread adoption (Wang *et al.,* 2019).
- Integration with Existing Systems: Overcoming technical challenges for integrating blockchain with legacy systems is essential (Gupta *et al.,* 2020).

5. Internet of Things (IoT)

The Internet of Things (IoT) represents a vast network of interconnected physical devices equipped with sensors and technologies that facilitate data collection and exchange. This review highlights critical innovations within IoT, its diverse applications, inherent challenges, and prospective developments. The Internet of Things (IoT) refers to the interconnected network of physical devices embedded with sensors, software, and other technologies that collect and exchange data over the internet. IoT enables these devices to communicate with each other and with centralized systems, facilitating automation, monitoring, and data analysis. Applications of IoT span various sectors, including smart homes, healthcare, agriculture, industrial automation, and smart cities,

enhancing efficiency, convenience, and decision-making. Key innovations in IoT include edge computing, which processes data closer to the source; the integration of artificial intelligence for improved data analysis; and advancements in connectivity through technologies like 5G. Despite its transformative potential, IoT faces challenges such as security vulnerabilities, interoperability issues, and energy consumption, necessitating ongoing innovations and robust frameworks to ensure safe and efficient deployment.

Innovations in IoT

- Edge Computing: This innovation allows data processing closer to its source, reducing latency and bandwidth use. It is particularly beneficial for real-time applications such as autonomous vehicles (Shi *et al.,* 2016).
- Artificial Intelligence and Machine Learning Integration : The combination of AI with IoT enhances data analysis and decision-making, enabling advanced functions like predictive maintenance (Zhao *et al.,* 2019).
- 5G Connectivity: The advent of 5G technology offers higher bandwidth and lower latency, significantly enhancing the capacity for connecting multiple IoT devices and supporting real-time data transfer (Zhang *et al.,* 2020).
- Blockchain Technology: Blockchain introduces a decentralized framework for securing IoT ecosystems, improving data integrity and enabling secure transactions (Iovan *et al.,* 2019).
- Interoperability Standards: Efforts towards standardization are vital for ensuring that diverse IoT devices can communicate effectively, promoting cohesive ecosystems (Gubbi *et al.,* 2013).

Applications of IoT innovations

- Smart Homes: Innovations in smart home technology enhance convenience and energy efficiency through devices like smart thermostats and security systems (Gao *et al.,* 2019).
- Industrial IoT (IIoT): In manufacturing, IoT facilitates real-time monitoring and predictive maintenance, leading to enhanced operational efficiency (Lee *et al.,* 2018).
- Healthcare: IoT devices enable remote monitoring and telemedicine, improving patient outcomes and reducing costs (Zhao *et al.,* 2020).
- Smart Cities: IoT technologies enhance urban living by optimizing resource management and improving traffic systems (Khan *et al.,* 2019).

- Agriculture: IoT innovations in agriculture enhance precision farming, optimizing resource usage and improving crop yields (Wolfert *et al.,* 2017).

Challenges and future directions

- Despite the advantages, several challenges remain:
- Security and Privacy: The proliferation of IoT devices raises significant security concerns, including data breaches (Zhang *et al.,* 2019).
- Scalability: The growing number of devices complicates data management and processing (Sethi & Gupta, 2017).
- Standardization: The absence of universal standards inhibits device interoperability (Gubbi *et al.,* 2013).
- Energy Consumption: Innovations in energy-efficient designs and energy harvesting technologies are necessary to address battery dependency (Zhao *et al.,* 2020).

Conclusion:

Artificial Intelligence (AI), Big Data, Blockchain, Cloud Computing, and the Internet of Things (IoT) represent innovative technological approaches that are fundamentally transforming industries by enhancing security, efficiency, and data-driven decision-making. However, these advancements come with challenges, including scalability issues, ethical dilemmas, and security risks. Future research should focus on addressing these obstacles while exploring new applications and fostering collaboration among these emerging technologies to create sustainable and future-ready solutions.

Continuous innovation in Big Data technologies is reshaping data management and analysis across industries. To fully harness its potential, challenges related to workforce skills, security, and privacy must be addressed through ongoing research and development. Advancements in Blockchain technology are driving improvements in efficiency, security, and transparency across various sectors. Despite facing hurdles, the prospects for widespread adoption and integration into everyday applications are promising.

IoT innovations are revolutionizing multiple industries by enhancing data-driven decision-making, automation, and connectivity. While challenges regarding security, scalability, and interoperability persist, recent developments indicate a significant potential for broader adoption of IoT technologies.

AI is rapidly evolving, driven by breakthroughs in deep learning, natural language processing, reinforcement learning, Edge AI, and explainable AI (XAI). This evolution brings

both practical and ethical challenges, with the future of intelligent systems dependent on effectively navigating these issues while seizing emerging opportunities.

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Innovative Approaches in Science and Technology Research Volume I
(ISBN: 978-81-979987-5-1)

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ISBN 978-81-979987-5-1
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