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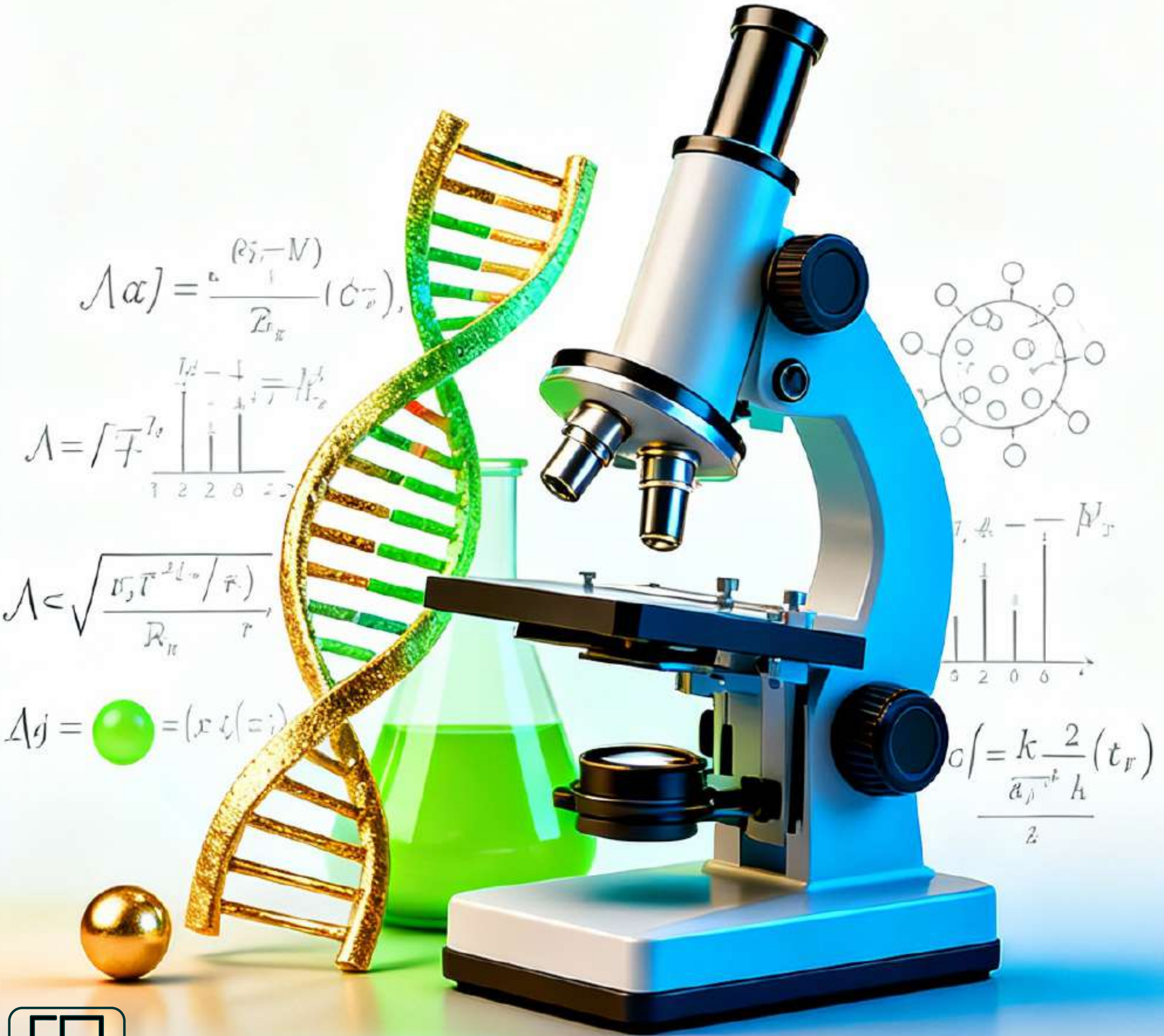

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Preface

This edited volume brings together a diverse collection of scholarly chapters that reflect the growing convergence of biological sciences, environmental studies, and mathematical frameworks in advancing modern research and innovation. Each contribution in this book highlights a unique dimension of interdisciplinary inquiry, offering readers both depth and breadth across multiple domains of contemporary science.

The opening chapters focus on the rapidly expanding field of bioinformatics, introducing essential tools and computational techniques that have transformed biological data analysis. Complementing this, the discussion on agricultural innovation and farming systems presents sustainable pathways to enhance productivity, resilience, and ecological balance—key priorities for global food security. Advancements in plant sciences and crop improvement technologies further underscore the importance of integrating biotechnology with traditional agricultural knowledge.

Environmental concerns take center stage in several chapters. The comprehensive review on the impact of water pollution on fish health and behaviour provides critical physiological and ecological insights relevant to aquatic conservation. Similarly, the chapter on plant bio-indicators offers an in-depth analysis of how vegetation can be used to monitor air, soil, and water pollution, strengthening environmental assessment strategies. The investigation into phytochemical profiling and ash analysis of Majidea zanguebarica adds a valuable dimension to natural product research and phytochemistry.

The book also includes significant contributions from the chemical sciences, particularly the chapter exploring phosphonium-mediated solvent extraction of copper, cadmium, and zinc, which sheds light on mechanistic pathways crucial for metal recovery and environmental remediation.

Recognising the universal language of mathematics, the final set of chapters explore its profound interdisciplinary applications. From semigroup theory to *mathematics as a bridge in higher education, these works highlight how mathematical thinking fosters analytical reasoning across disciplines. The chapter presenting a mathematical framework for ovarian follicle development and stimulation exemplifies the power of mathematical modelling in understanding complex biological processes.*

Together, these chapters represent a rich fusion of ideas, methodologies, and innovations. This book aims to serve as a valuable resource for researchers, educators, and students seeking to engage with interdisciplinary scientific research. It is our hope that the insights presented here will inspire further exploration, foster collaboration, and contribute to a deeper understanding of the interconnected nature of modern science.

Editors

Advances in Sciences and Allied Sciences

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Bioinformatics Basics: Tools and Techniques for Modern Biology

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Abstract

Data storage, accessibility, genomics, proteomics, and individualized treatment depend on biological databases in modern research. Researchers can easily access complex biological data from their huge biological data stores. By including biological data, public databases enable worldwide collaboration and tailored therapy to study genetic variation health effects. Nucleic acid, protein, and gene expression databases are needed due to the exponential development of biological data. In biotechnology, GenBank, DDBJ, and EMBL foster collaboration and research. Researchers utilize Entrez and BLAST to quickly retrieve and align sequences to study biological systems and pathologies. As the landscape evolves, these databases will aid information sharing and biological evolution.

Keywords: Nucleic acids sequences, protein sequences, GenBank, DDBJ, EMBL, Entrez and BLAST

Introduction

Biological databases play a crucial role in modern research by facilitating data storage, improving accessibility, and supporting advances in genomics, proteomics, and personalized medicine. These databases serve as repositories for large amounts of biological data, essential for researchers wishing to analyze and interpret complex biological information (Kumar, 2023). Structured storage of this data allows for efficient retrieval, ensuring that researchers have access to the information they need (Yekta & Arefi Oskouie, 2018). A database is a collection of relevant data related to certain aspects of the real world. Data mining is the technique of identifying hidden predictive information in large databases. Biology is no longer simply the study of living organisms. Every day, more and more scientists around the world create vast volumes of data (sequence, structure, etc.), and this data is growing at an exponential rate. Databases are becoming increasingly important in biological research, thanks in part to the rise of large-scale functional genomics and proteomics experiments focused on gene expression. These provide a wealth of information about each of the thousands of proteins that a genome codes for. Biological data are becoming increasingly diverse and numerous. As our understanding of biology has expanded, computer-based databases have become increasingly vital in this role.

Another key aspect of biological databases is accessibility. These public, user-friendly databases stimulate global scientific collaboration (Helmy, Crits-Christoph, & Bader, 2016). By making data easily accessible, researchers in genomics and proteomics may discuss, compare, and build on each other's work, accelerating development in these cutting-edge fields (Lapatas et al., 2015).

Biological databases also improve tailored medicine. They help integrate biological data to understand how genetic variants affect health and disease (Sharma & Yadav, 2022). Genomic and proteomic data allow researchers to personalize therapy to each patient's unique biological profile (Abugssaisa & Kasukawa, 2021). Personalization is crucial to patient outcomes and medical research.

In conclusion, biological databases improve modern research by efficiently storing and accessing biological data. They advance genomes and proteomics, enabling individualized treatment (Cannataro et al., 2014; Gray, 2022). These databases will become increasingly important in supporting scientific collaboration and innovation as biological data grows. Databases are required for grouping comparable sorts of data and creating a global network to access them, for example. SGD The Saccharomyces Genome Database contains all of the genomic and proteomic information on Saccharomyces. GenBank, EMBL, and DDBJ are large public databases containing nucleic acid sequences. PIR and SWISS-PROT include protein sequences, while the PDB (Protein Data Bank) stores three-dimensional protein structure coordinates. The sequencing data is also obtained using expressed sequence tags (ESTs) from cell lines. These tags are stored in dbEST, a GenBank component that provides information on how genes are expressed in various tissues. In addition to these generic data repositories, there are specialist databases such as SCOP, CATH, and FSSP that organize proteins based on their structural similarities. Pfam and ProtoMap, on the other hand, organize proteins based on how similar their sequences are. There have also been numerous databases created to provide complete access to sequence, structure, expression, functional data, and other information. Bioinformatics relies heavily on public-domain databases. Scientists enter data into these databases so that everyone can access it for free. This benefits everyone in the research community and allows them to complete their work faster. There are no strict guidelines for categorizing databases.

Databases can be broadly classified as

1. Sequence databases

2. Motif databases
3. Structural databases
4. Genome databases
5. Proteome databases
6. RNA expression
7. Others

Nucleic Acid Sequence Databases

The introduction of nucleic acid sequence databases has drastically altered the genetic research landscape, easing information exchange, promoting genomic discovery, and expanding biotechnology applications. At the center of this transition are databases controlled by organizations like the National Center for Biotechnology Information (NCBI), which is a valuable resource in this sector. NCBI provides comprehensive databases that enable academics to access a wide range of genomic and proteomic data, thereby enhancing joint research efforts (NCBI Resource Coordinators, 2012). The importance of such databases is growing as genetic information becomes more complicated and better data management is required. The three main nucleic acid sequence databases collect public sequences worldwide. These three databases share data every day. They depict the same entry in three versions. Any sequence submitted to one database appears in the other two. However, the three databases utilize distinct annotation formats and may have various cross-references.

One of the primary contributions of nucleic acid sequence databases is to facilitate information sharing, which is critical for collaborative scientific initiatives. Databases such as GenBank and the European Nucleotide Archive (ENA) save DNA and RNA sequences, allowing scientists from other fields to collaborate and build on one another's work (Sayers et al., 2010). This interconnection encourages a more holistic approach to biological research, allowing data sets to be merged and examined together. Many improvements in genetic research rely on the availability of previously published data, demonstrating the need of an open access approach (Diniz & Canduri, 2017). Furthermore, the use of bioinformatics databases has helped in genomic discovery, allowing the identification of novel genes, RNA sequences, and functional regions in genomes (Yan, 2008). Researchers use bioinformatics tools to perform sequence alignments, annotations, and phylogenetic analyses that would be time-consuming or impossible without these resources (Rehm, 2001). The combination of computational analysis with genetic data has led to advancements in comprehending complex diseases and hereditary features, representing a key milestone in genomics (Chen and Coppola, 2018).

The advancement of biotechnology applications has also been greatly affected by nucleic acid sequence databases. These resources help to create treatment strategies such as gene therapy and precision medicine, both of which require accurate genetic information to be implemented successfully (Lakshmi & Ramyachitra, 2020). As biotechnology advances, the ability to access and analyze large data sets becomes increasingly important, especially in situations requiring immediate decisions, such as identifying viral genomes during epidemics or personalizing treatments based on individual genetic profiles (Ismail, 2022). Furthermore, the increase of database resources has resulted in the development of specialized bioinformatics tools designed for specific biotechnological applications. For example, data mining algorithms on genomic datasets enable researchers to reveal previously unknown gene interactions, which can aid in drug discovery and development (Mukhopadhyay, Choudhary, & Iquebal, 2017). These developments emphasize the significance of bioinformatics as a link between raw data and practical applications in genetics and biotechnology. The ongoing development of internet databases and bioinformatics tools enables genetic researchers to analyze and interpret data with remarkable precision and speed.

The growth of sequence databases has not only increased research efficiency but also democratized access to genetic data across multiple research communities. This democratization promotes innovation by allowing researchers working in resource-constrained environments to interact with genomic data that would otherwise be unavailable (NCBI Resource Coordinators, 2015). The open access feature of these databases reduces inequities in research skills and helps to create a fairer worldwide research environment. As a result, collaboration across institutions and countries has increased, resulting in a more diverse interchange of knowledge and ideas that enhances scientific discovery. Finally, nucleic acid sequence databases have developed as critical components of genetic research, enabling information exchange, accelerating genomic discoveries, and propelling advances in biotechnology applications. As bioinformatics advances and databases grow, our ability to use genetic data effectively and efficiently will surely impact the future of genetics research and related fields, ushering in an era of tremendous scientific achievement. Integrating multiple data sets, expanding collaborative efforts, and developing globally available genomic information will all be critical as the scientific community attempts to better grasp the intricacies of life at the molecular level. These resources are both long-lasting and revolutionary, ushering in a new era of genomic research and technological development.

GenBank

GenBank, a key component of NCBI, has shaped genetic and biodiversity research since its founding. A major sequencing data store, it supports global bioinformatics infrastructure. GenBank's huge data sets and global scientific collaboration make it important. Genomic researchers can obtain and evaluate many nucleotide sequences from GenBank. This database is essential for basic research and advanced genomics. Regular updates and genetic material from varied organisms give scientists the latest data for their studies (Benson et al., 2014). For widespread sequencing data integration, NCBI has provided database resources with user-friendly interfaces (NCBI Resource Coordinators, 2012; Sayers et al., 2010). This accessibility helps researchers undertake comparative genomics, which is essential for understanding evolutionary linkages and functional genomics (Singh and Singh, 2015).

GenBank also strongly influences biodiversity research. Sequences from different species can be used to study genetic diversity and population organization (Yan, 2008). New species data and researcher contributions boost biodiversity databases (Mizrachi, McEntyre, & Ostell, 2007). Reference sequences enable phylogenomic research that informs conservation approaches and policy, stressing the database's role at the intersection of science and environmental awareness (Benson et al., 2012). GenBank also promotes worldwide scientific collaboration. Researchers from different countries can submit data and collaborate on genomic studies using an open access platform (Clark et al., 2016). Data democratization allows insights to be shared, examined, and improved across borders. GenBank's collaboration fosters interdisciplinary research, advancing ecology and medicine (Wheeler et al., 2001). This collaboration is essential for solving global issues like disease outbreaks and climate change, which require biological data insights.

Platforms like GenBank must evolve as researchers generate more sequencing data. Genomic databases need ongoing data curation and accessibility (Benson et al., 2012; NCBI Resource Coordinators, 2015). Thus, GenBank is a dynamic resource for genetic research and biodiversity conservation as well as a memorial to scientific progress. In conclusion, GenBank is essential to genomic research, biodiversity studies, and global scientific collaboration. Its evolution and responsiveness to scientific community requirements will boost its significance in approaching years.

DDBJ: The DNA Data Bank of Japan

The DNA Data Bank of Japan (DDBJ) advances genetic research, affecting biotechnology, bioinformatics, and personalized medicine. Along with SRA and ENA, DDBJ is a major genomic database. Its DNA sequence collection, storage, and sharing services benefit the global scientific community (Tateno et al., 2002). DDBJ can manage vast amounts of biological data, which is necessary for genomic investigations and research (Miyazaki et al., 2004). The DDBJ Omics Archive is notable. This resource allows functional genomics investigations, expanding bioinformatics research. Data of this size and organization allows scientists to explore complex genomic networks (Kodama et al., 2012). DDBJ makes these resources available to researchers to improve gene function and interaction understanding, which promotes biotechnology. DDBJ has grown and innovated throughout time. Update reports highlight database updates and enhancements to user experience and data accessibility (Tanizawa et al., 2023; Okido, 2022). The DDBJ data submission and retrieval methods have been greatly improved, making genomic data easier to access for researchers. International collaborative research has benefited from this (Mashima et al., 2016).

DDBJ integration with biological data streams increases research findings. This lets researchers compare data from different trials and studies to better understand genomics (Miyazaki et al., 2003). The database's strategic partnerships with mass sequencing teams enhance its capabilities and show its dedication to genetic research (Tateno et al., 2000). Comprehensive genomic databases like DDBJ are essential for personalized medicine, which tailors therapies to individual genetic profiles. DDBJ helps healthcare practitioners and researchers develop individualized treatments by giving open access to heterogeneous genetic data (Kodama et al., 2018). Analyzing individual genetic variations can lead to personalized therapy, improving patient care. Beyond hosting data, DDBJ supports global research efforts, highlighting its status as a biotechnology and bioinformatics leader. As genomic research evolves, the DDBJ will remain an essential resource, connecting genetic research to medical and technological applications.

EMBL: European Molecular Biology Laboratory

Through its efforts to promote scientific collaboration, technical innovation, and scientist training, the European Molecular Biology Laboratory (EMBL) has had a major impact on molecular biology research in Europe. Major contributions of EMBL include encouraging researcher collaboration. A platform for bioinformatics resources and cross-disciplinary interactions was established with the founding of the EMBL European Bioinformatics Institute (EMBL-EBI) (Thakur et al., 2023). In its many workshops and conferences, EMBL fosters collaboration, such as the European Conference on Computational Biology (ECCB), which brings European researchers together to share ideas, resources, and research projects (Kukkonen-Macchi et al., 2024). EMBL has also advanced molecular biology technology. EMBL has changed how scientists study human diseases and biology by using Big Data. Birney (2023) describes how EMBL's Big Data investments have helped researchers understand complex biological processes and improve data processing and interpretation. Technology infusion boosts Europe's research scene in structural biology, genomics, and proteomics beyond analytics (Cantelli et al., 2022). EMBL prioritizes teaching future scientists to keep research innovation going. The EMBL International Doctoral Programme and internships teach new researchers valuable skills (Manzano et al., 2023). Such programs ensure a consistent supply of qualified scientists to solve tomorrow's scientific concerns, reinforcing Europe's molecular biology research leadership.

EMBL promotes a lively scientific community through these training programs and by participating in projects that provide access to vital resources. The European Nucleotide Archive, managed by EMBL, provides nucleotide sequence data for European and international study. By giving more researchers access to high-quality data, open access resources boost European research visibility and impact. In conclusion, EMBL is the foundation of European molecular biology research, fostering collaboration, improving technology, and training future scientists. Its continued commitment to establishing an integrated research environment shows how these institutions promote scientific innovation and quality (Brunner et al., 2021; Cassata, 2024; Cassata and de Chadarevian, 2025). EMBL will shape European molecular biology and biomedicine as it evolves.

Protein Sequence Databases

Protein sequence databases have revolutionized bioinformatics and advanced genomics and proteomics research. Protein sequence databases store, retrieve, and analyse protein sequences, helping us understand biological activities and relationships. Bioinformatics tools can analyze DNA and protein sequences, assign gene functions, and classify proteins, according to Rehm (2001). Thus, they help researchers interpret complex biological data. Modern bioinformatics research requires data accessibility. Bioinformatics facilitates collaboration and innovation by enabling smooth access to large data sets, according to Diniz and Canduri (2017). Integrating genomic, transcriptomic, and proteomic data helps researchers understand molecular mechanisms and disease pathways. Gromiha (2011) underlines that protein bioinformatics can be used for sequence analysis and functional predictions, showing how data sets can reveal protein functionality. The rise of bioinformatics databases has also affected virology. In virological research, these databases provide crucial information on viral protein sequences and host organism interactions, according to Yan (2008). Such data enhances viral biology knowledge and aids treatment development. According to Lakshmi and Ramyachitra (2020), bioinformatics tools have converged, improving sequence alignment, docking, and drug discovery, simplifying proteomics research. Chen, Huang, and Wu (2010) say protein sequence databases integrate and standardize data. These databases aid comparative proteomics by identifying comparable proteins across species. This comparative technique assists functional annotation and evolutionary studies, tracing protein family evolution. Sharma, Sharma, and Sharma (2019) present a comprehensive bioinformatics overview that supports the idea that researchers need well-organized protein data to generate new discoveries.

The history of bioinformatics shows ongoing data management evolution. Gauthier et al. (2019) describe how computational tools and robust databases have accelerated protein analysis, enhancing scientific research. Genomic and proteomics advancement depends on excellent data management as bioinformatics evolves. Persson (2000) further supports the idea that bioinformatics is essential to protein analysis by offering tools to evaluate protein structures and functions. These integrated methods allow researchers to unlock protein sequences' potential, advancing scientific sectors. Finally, Jiménez-López et al. (2013)'s comprehensive compilation of bioinformatics tools and databases emphasizes the need for systematic approaches to analyze genomic and proteomic data sets and protein sequence databases in bioinformatics research.

Amino acid sequences are derived from the translation of nucleic acid sequences. In contrast to nucleotide sequence databases that contain identical sequence data, the principal public protein sequence databases each possess distinct characteristics. The subsequent are the principal protein sequence databases:

SWISS-PROT (SwissProtein)

SWISS-PROT, a protein knowledge database, has advanced bioinformatics by providing reliable and complete functional protein information. SWISS-PROT, started under UniProt, features accurately annotated entries by experienced editors (Gasteiger, Jung, & Bairoch, 2001). Apweiler (2001) noted that SWISS-PROT's functional information provides a solid foundation for large-scale protein sequence characterisation due to its rigorous curation process. Beyond sequencing data, SWISS-PROT provides insights on protein families, domains, and post-translational modifications that are vital for understanding protein function and interaction networks. The SIB Swiss Institute of Bioinformatics recommends SWISS-PROT for academics investigating curated databases that aid biological research (SIB Members, 2016). These advances have transformed bioinformatics research, enabling more complex studies that account for protein activity's biological environment (Boeckmann et al., 2005).

SWISS-PROT is more useful when combined with other datasets and technologies. The UniProtR framework speeds up protein sequence and functional data retrieval and visualization, improving researcher experience (Soudy et al., 2020). SWISS-MODEL, based on SWISS-PROT, also improves structural bioinformatics (Bienert et al., 2017). These technologies allow scientists to study protein functions and functionally similar proteins in different animals. SWISS-PROT is notably influential in drug discovery. Comprehensive functional annotations help researchers find therapeutic targets and understand drug processes (Edwards & Cottage, 2003). This is crucial for developing new

therapeutic methods, especially in areas where functional understanding is lacking. In biomedical research, SWISS-PROT's ability to resolve conflicts amongst databases, including GenBank, makes it reliable. Karp, Paley, and Zhu (2001) found this.
SWISS-PdbViewer and other automated tools and frameworks from SWISS-PROT demonstrate its lasting impact on comparative modeling and structural bioinformatics (Guex, Peitsch, & Schwede, 2009). These methods improve predictive modeling and 3D structural analysis for protein functional annotation, improving our understanding of protein dynamics in a biological context. In conclusion, SWISS-PROT remains an essential protein knowledge database resource for bioinformatics and functional annotation. His work impacts biological research and drug discovery, demonstrating the importance of reliable and complete protein data (Schneider, Tognolli, & Bairoch, 2004). The expanding discipline emphasizes SWISS-PROT's importance in understanding biology and disease.

SWISS-PROT incorporates:

- Function of the protein
- Post-translational modification
- Domains and sites.
- Secondary structure.
- Quaternary structure.
- Similarities to other proteins;
- Diseases associated with deficiencies in the protein
- Sequence conflicts, variants, etc.

PIR-PSD

The 1984 founding of the Protein Information Resource (PIR) by the National Biomedical Research Foundation (NBRF) laid the groundwork for a comprehensive scientific database. This endeavor began due to the growing need for standardized protein sequence data. Since its founding, PIR has sought to make protein sequence information more accessible and usable, enhancing biology and medicine research (Barker et al., 1992). PIR is an international protein sequencing database that collects, organizes, and distributes data. Barker et al. (1998) say the database helps protein sequence research by offering easy access to substantial data for functional genomics and proteomics. PIR helps researchers comprehend protein function and structure by allowing comparative examination of newly sequenced and previously described proteins (George et al., 1987). PIR has been improved over time to be more useful. George and Hunt (2012) show how this resource has evolved, including the addition of data analysis bioinformatics tools. This has increased protein science research opportunities and fostered collaboration. PIR benefits protein researchers at Georgetown University Medical Center, where protein research is emphasized.

Collaborations with other protein databases and large-scale annotation efforts have confirmed PIR's data and strengthened its credibility in protein research (Wu, 2003). These collaborations have refined data sets, enabling key findings that advance medical research, notably molecular disease knowledge. Barker et al. (1999) show how PIR has improved data format for bioinformatics integration. According to Kehoe (2019), specialized databases like PIR allow researchers to ask complicated biological questions and better understand molecular activities through comparative sequencing analysis. This enriches molecular biology and promotes multidisciplinary study. Ludwig (1995) noted that protein sequence databases have altered molecular biology over time. Today's protein sequence analysis and characterization relies on PIR's early methods (Sivakumar, 2007). This crucial PIR work shows how devoted resources promote scientific research and advance human knowledge. The 1984 founding and development of the Protein Information Resource by NBRF has had major effects on protein research and the scientific community. The usage of PIR by Georgetown University Medical Center reinforces its importance in protein science and related domains.

The majority of PIR sequences also appear in the Swiss-Prot database, and vice versa. The PIR database contains annotated sequences, although the annotations differ from those of SWISSPROT sequences. PIR formed the UniProt consortium in 2002 in collaboration with the European Bioinformatics Institute (EBI) and the Swiss Institute of Bioinformatics (SIB). PIR-PSD sequences and annotations have been added to the UniProt knowledgebase. Bidirectional cross-references between UniProt (UniProt Knowledgebase and/or UniParc) and PIR-PSD have been created to make it easier to search down old PIR-PSD entries.

UniProt (Universal Protein resource)

UniProt is used in protein research to retrieve data, annotate functions, and develop bioinformatics and personalized medicine. UniProt, a global standard for protein sequence and function data, offers researchers a wealth of protein information (Bairoch et al., 2005). Data accessibility provided by UniProt is critical. The platform enables professionals from all across the world to easily retrieve protein sequences, functional data, and other information for proteomics and genomics research. In 2010, the UniProt Consortium reported more than 18 million protein sequences, confirming its position as the leading protein data repository. UniProt has been updated and modified to address the growing demand for organized and accessible protein information based on genetic data (UniProt Consortium, 2009). UniProt functional annotation is also critical for determining protein biological roles in various animals. UniProt uses both automated and manual annotation to ensure complete and trustworthy data. The integration of enzyme activity, sickness connections, and biological pathways has advanced both scientific and applied research (UniProt Consortium, 2014). This functional annotation is required to identify protein functions in diseases, which has implications for personalized therapy.

In bioinformatics and personalized medicine, integrating protein data with genomic, transcriptomic, and metabolomic data is critical. UniProt contributes to this. Protein function association with patient variables allows for personalized treatment choices (UniProt Consortium, 2012). UniProt data has been used to identify biomarkers and medicinal targets, resulting in improved therapeutic accuracy (UniProt Consortium, 2010). In its activity report, the UniProt Consortium highlighted its data space restructuring as a means of improving information retrieval and remaining relevant. This includes utilizing more sophisticated computer tools for data retrieval and processing. UniProt remains at the vanguard of bioinformatics due to advancements in database design and functionality, which match the growing demand for efficient and systematic protein data handling. Finally, UniProt facilitates protein research data access, provides precise functional annotations, and promotes bioinformatics and personalized medicine. As proteomics advances, UniProt's data management and dissemination will contribute to a better understanding of protein activities and their consequences on health and illness.

ENTREZ: Dedicated Tools of Retrieving a Biological Data

Entrez is a web-based data retrieval tool created by the NCBI, enabling searches across 11 integrated NCBI databases, including GenBank and its subsidiaries, OMIM, and the literature database MEDLINE via PubMED.

Entrez is accessible through the NCBI webpage and is an intuitive, user-friendly platform. Text search phrases facilitate the querying of individual databases, whereas sequences can serve as queries in tools like BLAST. Hits are organized by relevance or similarity, with hits on the target database referred to as neighbors and hits on other databases termed connections.

The NCBI is a component of the National Library of Medicine (NLM), which is a division of the National Institutes of Health (NIH) in the United States. Entrez is the French second person plural (or formal) form of the verb "to enter," signifying "come in."

Entrez Global Query is a unified search and retrieval system that enables simultaneous access to all databases through a single query string and user interface. Entrez can effectively obtain associated sequences, structures, and references. The Entrez system offers access to gene and protein sequences as well as chromosome maps. Certain textbooks are accessible online via the Entrez system.

Entrez serves as the unified interface for all databases managed by the NCBI and is remarkably user-friendly. The searchable databases can be accessed via hyperlinks at the top of the page or through the shown drop-down menu. After selecting a database, a search term is entered in the designated field. The query may consist of a singular term or a Boolean expression. Clicking 'GO' commences the search. Records in the chosen database are presented (termed as neighbors), together with corresponding entries in other Entrez databases (referred to as connections). Hits are arranged by similarity according to precomputed analyses of sequences/structures or existing literature.

Entrez additionally offers a comparable interface for querying individual databases and for honing search outcomes. The Limits feature enables the user to refine a search within a web forms interface. The History feature provides a sequential enumeration of recently executed searches. Results from prior queries can be referenced by number and amalgamated using boolean operators. Search results may be temporarily stored in a Clipboard.

Besides utilizing the search engine forms to query data in Entrez, NCBI offers the Entrez Programming Utilities (eUtils) for more direct access to query outcomes. The eUtils are accessed by submitting specifically structured URLs to the NCBI server and interpreting the XML response. An eUtils SOAP interface is also available.

BLAST (Basic Local Alignment Search Tool)

The Basic Local Alignment Search Tool (BLAST) has fundamentally transformed the field of bioinformatics since its introduction. This computer algorithm allows researchers to quickly and efficiently compare biological sequence information, including DNA, RNA, and protein sequences. The rapid alignment capabilities of BLAST have become indispensable in genomics, contributing greatly to scientific progress and our understanding of various diseases (Madden, 2013). Analyzing the impact of BLAST on bioinformatics, we can see its complex relationship with algorithmic development, applications in genomics and contributions to ongoing research. At the heart of BLAST's effectiveness are its algorithms, which use a heuristic approach to find regions of local similarity between sequences. The heuristic nature of BLAST means that it sacrifices some precision for speed, allowing it to handle large data sets that would be impossible to compute with exact algorithms (Korf, Yandell, & Bedell, 2003). Notably, the algorithm identifies high-scoring segment pairs (HSPs) as an initial step before extending the alignment, thereby optimizing the calculation process (Gupta & Rani, 2010). As a result, BLAST has paved the way for further advances in algorithm design, inspiring variants such as BLAT (BLAST-Like Alignment Tool) and TBLASTN, which facilitate sequence comparisons under different parameters (Gupta, 2017).

The application of BLAST extends significantly to genomics, where it serves as a fundamental tool for gene annotation and comparative genomics. For example, researchers frequently use BLAST to identify homologous genes in various species, which can provide insight into evolutionary relationships and functional predictions (Diniz & Canduri, 2017). Its application in large-scale genomics projects, such as the Human Genome Project, illustrates BLAST's ability to efficiently manage and analyze large sequence data (Kapetanovic, Rosenfeld, & Izmirlian, 2004). Additionally, innovations in BLAST technology, such as the implementation of BLASTGrabber, enhance its functionality by allowing users to visualize and analyze substantial amounts of output data, making it more accessible to research communities (Neumann, Kumar, Haverkamp, & Shalchian-Tabrizi, 2014).

BLAST's role in scientific research and understanding of diseases is also profound. By enabling the identification of conserved sequences involved in disease mechanisms, researchers can target these sequences for further analysis or therapeutic intervention. For example, the application of BLAST has been essential for identifying genes associated with genetic disorders and infectious diseases, as it facilitates the comparison of pathogen genomes with human host sequences, providing insight into mechanisms of pathogenicity and resistance (Samal et al., 2021). Additionally, the integration of computational techniques such as BLAST in areas such as chemoinformatics has led to new applications in drug design and development. By leveraging sequence data, researchers can identify potential drug targets by finding analogous sequences with known functions (Arora & Malik, 2021).

Technological advancements that support BLAST tools have also evolved significantly to improve computing performance. Projects such as ScalaBLAST have emerged, focused on scalable implementations suited to the ever-increasing volume of genomic data (Oehmen & Nieplocha, 2006). These high-performance adaptations allow researchers to conduct analyzes that were previously inaccessible due to processing power limitations. Additionally, ongoing updates to the NCBI BLAST toolbox ensure that researchers have the latest tools and optimizations for sequence alignment, significantly influencing the direction of bioinformatics research (Neumann, Kumar, & Shalchian-Tabrizi, 2014).

In education, BLAST serves as an introductory tool for students entering bioinformatics. Numerous studies have documented its effectiveness as a learning resource, providing accessible ways for novices to engage in biological data analysis (Syngai, Barman, Bharali, & Dey, 2013). Educational initiatives incorporating the use of BLAST have facilitated a better understanding of sequence alignment principles among students and early career researchers. The wealth of applications highlighted by BLAST highlights its essential role in bioinformatics as a versatile tool that shapes scientific research and contributes to a comprehensive understanding of biological sequences. As the field of genomics continues to evolve, the methods and heuristics underlying BLAST will likely spur further technological improvements, pushing the boundaries of genomics research. This, in turn, will have crucial implications for our understanding of complex biological systems and the advancement of personalized medicine through better disease diagnosis and treatment options (Mount, 2007; Schmidt, 2003). In summary, BLAST has a significant and diverse influence on bioinformatics, as evidenced by its cutting-edge algorithms, wide range of genomic applications, and vital contributions to scientific study. The alignment tool will continue to be the foundation of genetic analysis and a driving force behind comprehending the complexities of life at the molecular level as long as scientists continue to take use of its potential. It is clear that as the field develops, BLAST will not only remain relevant but also change to accommodate the demands of a biological environment that is becoming more and more data-driven (Sharma, Dhar, & Kaul, 2012; Lavenier & Giraud, 2005; Taylor, 2010).

Summary

Biological databases are pivotal in contemporary research, enhancing data storage, accessibility, and advancements in genomics, proteomics, and personalized medicine. They function as repositories for extensive biological data, allowing efficient retrieval for researchers analyzing complex biological information. Public databases facilitate global collaboration, while also supporting individualized therapeutic approaches by integrating biological data to discern how genetic variants impact health. The exponential growth of biological data necessitates the continued evolution of databases, which now include specialized types for various aspects such as nucleic acids, protein sequences, and gene expression. Key repositories include GenBank, DDBJ, and EMBL, which collectively contribute to collaborative scientific efforts and technological advancements in fields like biotechnology. Tools such as Entrez and BLAST further support researchers by enabling efficient data retrieval and sequence alignment, significantly impacting the understanding of biological mechanisms and disease. As the landscape evolves, these databases will continue to be crucial for facilitating knowledge exchange and enhancing biomedicine.

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Agricultural Innovation in Farming Systems: Pathways to Sustainable and Resilient Production

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Abstract

Agricultural innovation in farming systems is increasingly recognised as essential to address challenges of food security, climate change, resource scarcity, and sustainable development. This chapter reviews key dimensions of innovation in farming systems—including technological, organisational, and institutional innovations—and examines how they are embedded in farming systems through the lens of the Agricultural Innovation Systems (AIS) framework. Major innovations such as precision agriculture, climate-smart farming, digitalisation (IoT, AI), circular and agro-ecological systems, and organisational models like farmer producer organisations are discussed. Adoption barriers, enablers, policy, and institutional frameworks are also explored. The chapter concludes with recommendations for policy, research, and practice.

Keywords: Agricultural innovation, precision agriculture, climate-smart farming, digital agriculture, sustainable farming.

Introduction

Farming systems worldwide face pressures from population growth, changing diets, climate variability, declining natural resources, and evolving policy regimes. Innovation in agriculture—encompassing technical, organisational, and institutional change—is critical to increase productivity, enhance resilience, optimise resource use, and promote sustainability.

Conceptualising Innovation in Farming Systems

- **Role of Innovation in Sustainable Agriculture**
  Innovation is key to addressing the complex challenges of modern agriculture. Sustainable agriculture requires improved productivity, efficient use of resources, resilience to climate change, and environmental conservation. Innovations in crops, technology, management practices, and policy frameworks contribute to these objectives.

- **Evolution of Farming Systems**
  Farming systems have evolved from traditional subsistence practices to intensive and diversified production systems. Technological progress, market integration, and institutional reforms have shaped modern farming systems. The Agricultural Innovation Systems (AIS) framework highlights the importance of interactions among farmers, research institutions, extension services, private sector, and policymakers in promoting innovation.

Key Innovation Pathways in Modern Farming Systems

- **Precision and Digital Agriculture**
  Precision agriculture and digital tools, including sensors, IoT, drones, and AI, enable site-specific management, real-time monitoring, and data-driven decisions. These technologies can increase yield, reduce resource use, and enhance environmental sustainability. Adoption is influenced by cost, technical knowledge, and access to digital infrastructure.

- **Climate-Smart and Smart Farming**
  Climate-smart agriculture integrates adaptation and mitigation strategies to cope with climate variability. Practices include drought-tolerant crop varieties, efficient irrigation, conservation tillage, integrated pest management, and renewable energy use. Smart farming leverages digital tools to enhance efficiency and decision-making.

- **Agro-Ecological and Circular Farming Models**
  Agro-ecological approaches emphasise biodiversity, soil health, and ecosystem services. Circular farming aims to reduce waste, recycle nutrients, and close loops in farm systems. Such approaches contribute to long-term sustainability and resilience.

Table 1. Selected Agricultural Innovations and Impacts

Innovation	Function	Impact
IoT-based irrigation	Soil moisture monitoring	Up to 25% increase in productivity
Drones/UAV crop monitoring	Mapping & pest detection	Water use reduction up to 90%
AI decision tools	Yield prediction, disease diagnosis	>90% accuracy in disease diagnosis

Adoption, Barriers and Enablers

- **Socio-Economic Drivers of Innovation**
  Adoption of innovations is influenced by farm size, resource availability, education, digital literacy, access to extension services, credit, and market incentives.

- **Barriers and Risk Perception**
  Barriers include high initial costs, technical complexity, lack of training, risk aversion, inadequate infrastructure, and weak institutional support. Addressing these barriers is essential for broader uptake.

- **Enablers and Support Mechanisms**
  Enablers include participatory innovation, farmer co-design of technologies, capacity building, financing schemes, policy incentives, and strong extension networks.

Institutional and Policy Frameworks

- **Policy and Governance**
  Governments and public agencies shape innovation through R&D funding, extension, infrastructure development, and regulatory frameworks. Effective governance promotes innovation creation, diffusion, and scaling.

- **Building Innovation Ecosystems**
  Innovation ecosystems connect research institutions, private sector, farmers, advisory services, and financial institutions. Collaborative networks enhance knowledge flow, technology transfer, and adoption.

Implications for Developing Countries

- **Inclusive Innovation for Smallholders**
  Smallholders face structural constraints such as small farm size, limited capital, and weak extension. Inclusive innovation ensures access to new technologies, knowledge, and markets for women, youth, and marginalized groups.

- **Sustainability and Resilience**
  Innovations must balance productivity, environmental sustainability, and social equity. Integrated approaches enhance resilience to climate shocks and long-term viability of farming systems.

Conclusion

Innovation in farming systems transforms how agriculture operates, is organised, and governed. Technological, organisational, and institutional innovations within the AIS framework can enhance productivity, sustainability, and inclusiveness. Policies, extension, and collaborative networks are critical enablers for scaling and sustaining these innovations.

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Plant Sciences and Crop Improvement Technologies

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Abstract

Plant sciences and crop improvement technology focus on genetically modified plants using traditional breeding programs genomics and gene editing to achieve traits like yield nutritional value and biotic and abiotic stress resistance in plant. Advanced genomics and tools like CRISPR/Cas9 are used for faster improvements as compared to traditional breeding methods. Key areas include molecular techniques useful for understanding plant genome improving crop residences to different environmental factors like drought and salinity. Development in crop can be achieved using technology like precision agriculture and machineries to monitor crops and apply resources efficiently.

Keywords: Genetically modified plants, CRISPR, Cas9, traditional breeding, precision agriculture.

Introduction

Plant science and crop improvement technologies are important areas in sustainable agriculture, responding to the increasing food demand that can be seen globally due to climate change. Considering environmental impact, there have been current achievements and many advancements have rapidly evolved in the field of agriculture, including synthetic biology, epigenetics, and metabolism. These are the transformative solutions for enhancing crop production yield nutrient uptake in plant as well as stress tolerance in plant which maybe biotic and abiotic stress however their novelty also requires a wide comprehensive evaluation with their application and also for safety implications.

Crop improvement is essential to attend food security and enhancement of nutrition for human beings in worldwide, for a long-time conventional breeding has contributed towards crop improvement but in the last three decades the revolution of molecular breeding has arrived in crop improvement. The traditional crop improvement methods are working but unable to fulfil the demand of growing population. The advancement in molecular techniques such as TALENs, ZFNs and CRISPR came into the picture to provide more specificity. The genetic engineering including transgenic facilitates the transfer of desired characters into other plants which is not possible through conventional plant breeding programs, through genetic engineering the development of several crop plants that are resistant to biotic and abiotic stresses as well as herbicide tolerance are carried out.

GM crops cultivated includes tomatoes with alfalfa, rice, soya been, canola, brinjal, tobacco cotton, sugar beets, sweet pepper and carnations. Apart from food resources GM crops are used to remove heavy metals from the soil which can rehabilitate waste land for use in agriculture (Nishat P., 2020).

Plant Sciences

Plant science is a field of biology focusing on understanding plant life and also the interaction with the environmental factors whereas crop improvement technologies are the practical application of plant science knowledge to overcome agriculture productivity the quality of crop product and resilience plant science and compasses many disciplines in all aspects of plant life from cellular function to ecosystem level (Nishat., 2020)

Key areas of the study include:

- **Plant Physiology:** It is defined as the study of plant functions including photosynthesis respiration nutrient uptake and hormonal functions.
- **Plant Genetics and Genomics:** It is a field of biology which studies the inheritance of traits genetic makeup of the plant and use of DNA sequence to identify gene of interest.
- **Plant Pathology:** Plant pathology deals with the investigation and management of plant diseases caused by pathogens like viruses, bacteria and fungi etc.
- **Plant Ecology:** Plant ecology is the interaction between plant and environmental factors as well as other organisms and their role in nutrient cycling and climate regulation.
- **Biochemistry and Molecular Biology:** Biochemistry and molecular biology deals with the chemical processes and molecular mechanism inside a plant cell.

Crop Improvement Technologies

Crop improvement technologies and plant science are interrelated crop improvement technologies grip knowledge from plant sciences and its branches to develop new varieties with desirable trait of interest including disease resistant crops, higher yield, early maturity and quality products. There are several crop improvement methods ranging from traditional selection processes to genetic engineering technology.

Technologies Used in Crop Improvement

a. **Domestication and Selection:** Domestication is a historical process of modifying wild varieties of plants to produce desirable traits (A. Chinthiya,2019). Selection is the process of choosing a plant with desirable characters used for gene modification.

b. **Cross Breeding and Hybridization:** Cross breeding and hybridization are different cross breeding involves cross pollinating different varieties to combine favourable traits a method which has gained systematic application and also the understanding of mendelee and gene.

c. **Mutation Breeding:** Mutation breeding deals with the use of mutagens which may be physical and chemical mutagens to induce genetic variation followed by selection of desirable traits.

d. **Tissue Culture:** Plants are grown under artificial conditions it is also called as in vitro growth of plantation which requires controlled medium for the regeneration of entire plant which is used for micro propagation and generating variation.

Modern and Advance Technology

Genetic Engineering/Transgenics: The foreign DNA is isolated and introduced in the plant of interest to confirm specific traits such as insect resistance or herbicide tolerance (Nikhil., 2023)

- **Insect Resistant Crops.**
  BT cotton/maize/brinjal- beti cotton maize corn contains crying isolated from bacillus thuring genesis BT the protein produced is harmless to human and beneficial against insect in alkaline gut of certain pests. (Cotton ballworm and brinjal shoot borers), it becomes active and kill insect at larval stage.

- **Herbicide Tolerant Crops:** Modified to withstand specific broad spectrum herbicide allowing farmers to control weeds without harming crops.
  Example: Roundup ready soya bean/canola/corn/sugarbeets, crops have aroA gene inserted from Salmonella typhimurium that make them resistant to herbicide glyphosphate the active ingredient in products like round up.

- **Nutritional Enhancement:** These are designed to improve nutritional content of food addressing dietary deficiency in certain population.
  Example:
  1. **Golden Rice:** Rice variety has been engineered by inserting two jeans one from daffodil and one from micro to produce beta carotene precursor of

Vitamin C which will enhance the rice quality and nutritional content (Al-babili., 2005).

2. Pink Pineapple: GMO pineapple was developed to help pink flash by increasing levels of lycopene the pigment that makes tomato and watermelon pink.

- **Genome Editing:** Technologies precisely used in genome editing which includes CRISPR/Cas9/ZFNs (Zinc finger nickases) and TALENs which allow targeted modification in plant DNA to improve traits like diseases resistant, drought tolerance, nutrient content (Asadollah., 2025)
  ZFNs are the proteins used in genome editing which will induce double standard break in DNA as per target site. They are modified to create single standard break our neck rather than double strand break.
  TALENs talents are widely used in varieties of organism ranging from plant to human. TALENs are used to engineer disease resistance in wheat and rice and to improve quality of oil in soya bean which can be achieved by modifying FAD2 gene to increase oleic acid content (Aayashi., 2023)

- **Diseases and Spoilage Resistant Crops:** These plants are modified for the resistance of specific diseases or slow down the ripening process reducing the food wastage.
  1. **Virus Resistant Papaya:** In Hawaii the papaya industry was nearly destroyed by ring spot virus in 1990 or transgenic papaya variety called rainbow papaya was developed with the gene from virus coat protein making it resistant to disease and saving the industry from loss.
  2. **Flavr Savr Tomato:** The first commercial grown transgenic plant which was introduced in 19 94 and it was clever saver tomato which is modified with an antisense gene which can delay the ripening process and extend the shelf Life by interfering with enzyme polygalactonurase.

- **Omics technology:** Omics is the combined study of genomics, transcriptomics metabolomics and proteonomics used in comprehensive understanding of plant function at molecular level helping to identify target for improvement (Kumar., 2025)

Other examples of omic application in plant research

1. **Genomics:** Genomics leaves in identify single nucleotide polymer link trait like yield in pigeon pea etc (Bhattacharjee., 2021)
2. **Transcriptomics:** The real time changes in green expression while under stress condition which includes hit stress to reveal how plants adaptive and survive under adverse climatic conditions (Ainley., 2013)

3. **Metabolomics:** Metabolites such as flavonoids and stress related phytohormones that are produced and modified during stress are studied under metabolomics (Thillani., 2024).
4. **Epigenomics:** Study of DNA methylation which affects gene expression and consequently responsible for plant trait and adaptability under such conditions regards to plant response.
   Example: Ginseng response to cold temperature.
5. **Metagenomics:** Microbial community is present in or inside the plant are analysed under metagenomics.
6. **Proteonomics:** The abundance modification and interrelation of proteins were analysed and understand for their role in plant response to stress (Ahmad., 2016)

- **Precision Agriculture**

The data driven approach to farming which uses technology for management of crop and soil with side specific accuracy rather than treating entire field uniformly. Different tools like GPS drones sensors are used to collect data and apply inputs like water fertilizer and pests, where and when ever it is needed (Che Hau., 2024)

Key Technology Include

1. **Global Positioning System (GPS):** GPS precisely provides location data for navigation mapping and guidance of machineries.
2. **Drones And Satellite Imagery:** Crop growth can be monitor ed using aerial data which will lead to identify problem areas and access field conditions.
3. **Soil Sensors:** Soil properties like moisture and nutrient levels pH can be measured using soil sensors.
4. **Yield Monitors:** Measuring yield green moisture and other data is possible by installing yield monitors on harvesters while harvesting the crops.
5. **Variable Rate Technology:** VRI is a system of sensor and controller that automatically edges the application of inputs in the field.

- **Other Notable Examples**

1. **Production of Pharmaceuticals:** Exploration of transgenic plants as a bio reactor for production of valuable proteins which may include antibodies which is further used for medical purpose this process is known as molecular farming.
2. **Salt Tolerant Plants:** Salt tolerant species like mangroves were used by the researchers to produce plants to be more tolerant to high soil salinity by transferring gene of interest.

Goals of Crop Improvement Technologies

1. **Increased Agriculture Productivity and Yield:** Maximum yield per unit area by development of new crop varieties and hybrid hybrids to meet global population demand.
2. **Improve Resources Use Efficiency:** Plant deficiency can be enhance using essential resources like water nutrients and light.
3. **Shorten and Growth Duration:** Early maturing varieties can be developed and allowed it for multiplication in different cropping season within a year which will overcome productivity.
4. **Enhancing Quality and Nutritional Value:** End to end product quality improvement will enhance desirable traits such as grain size colour milling baking qualities in wheat cooking quality in rice and fibre quality in cotton
5. **Boost Nutritional Content:** The bio fortification leads to increase the level of important nutrients like proteins vitamins and different type of mineral contents which will tackle malnutrition's issues.
6. **Eliminate Toxic Substances:** The natural occurring toxic compounds can be reduced or removed naturally which are present in certain crops to make them safe for human consumption.
7. **Improve Postharvest Quality and Shelf Life:** The durability and keeping quality of fruits vegetables and grains to reduce food loss and wastage in supply chain can be enhanced.

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Impact of Water Pollution on Fish Health and Behavior: A Review of Physiological and Ecological Consequence

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Abstract

Water pollution is a significant environmental concern which has a negative effect on aquatic environment especially fish populations. Fish play very important roles in the health of aquatic environment and also as bioindicators in water quality. Contamination of water bodies, which may include heavy metals and pesticides, pharmaceutical and organic contaminants, and so on, may cause a considerable change in fish health and behavior, with short-term and long-term ecological effects.

Examples of such heavy metals include mercury, cadmium and lead and they build up in fish muscles and lead to various physiological disturbances such as neurological impairments, liver dysfunction and immune malfunction. Any buildup of these pollutants not only causes direct damage to the fish, but also has indirect effects on the food chain as a result of bioaccumulation. Likewise, all those pesticides and pharmaceuticals found in agricultural and urban runoff can interfere with the hormonal and neurological systems of fish and cause changes in feeding behavior, reproductive failures, and diminished antipredator behavior.

Further, organic pollutants, such as petroleum hydrocarbons and nutrient pollution, cause hypoxic effects in water bodies and suffocating aquatic life and preventing fish population growth and reproduction. These problems are further worsened by eutrophication which is instigated by the volume of nutrient runoff which further contributes to harmful algal blooms which further worsen the water quality.

Other typical effects of pollution include behavioral changes in fish including disturbed swimming behavior, impaired social interactions as well as reduced foraging effectiveness. Such behavioral disorders may make them prone to predations, lower the chances of reproductive success, and long-range survival of

fish populations.
The paper is a review of the different pollutants that impact on the health and behavior of fish and it has been noted that there are physiological and behavioral changes as a result of various forms of pollution. This paper has highlighted the necessity of combating the problem of water quality to promote the health and viability of aquatic ecosystem based on the comprehensive effects of pollution on fish.

Keywords: Water pollution, bioaccumulation, pharmaceuticals, aquatic ecosystem.

Introduction

One of the most widespread environmental problems in the world today is water pollution in aquatic ecosystems. As the world has been rapidly industrializing, urbanizing, and intensifying agriculture, the quality of the water bodies such as rivers, lakes and oceans has been degraded so much in the last century. Industrial effluents, agricultural runoffs, untreated sewage, and domestic wastes are some of the various sources of pollutants that infiltrate water bodies resulting in various adverse effects. These pollutants consist of heavy metals, pesticids, pharmaceuticals, plastics and organic compounds and each of them has a specific hazard to aquatic life, particularly, fish. Fish belong to the most susceptible species that are exposed to water pollution because they come into direct contact with their water environment. Fish being ectothermic creatures are very delicate with regard to water quality, temperature and chemical composition. Fish populations can cause cascading impacts to the whole ecosystem since they play an ecological role in the aquatic food webs. Fish are a resource of great ecological value as well as a vital bioindicator of the health of the aquatic environment. Their health and behaviour can be used to determine the extent of pollution and general well-being of water bodies (Scott and Sloman, 2004).

The health alterations in fishes brought about by pollution are complex and constitute physiological and behavioral effects. Physically, pollutants may affect the functioning of the vital organs, e.g. liver, gills, and kidney, with heavy metals, and endocrine-disrupting chemicals interfering with its functionality. These toxins lead to chronic toxicity, which is usually acquired over time, as it is accumulated in fish tissues, which makes fish prone to diseases, and leads to the weakening of their immune systems. Furthermore, the pollutants may interfere with fish development, procreation, and metabolism resulting in decreased mortality rates and decline in the population density. Besides affecting the physiology of fish, pollutants may also result in behavioral changes among fish. Such shifts in the behavior, though relatively minor, may have far-reaching effects on the population and survival of fish. Fish can get affected by pollutants on their cognition including learning and memory, decision-making. The effects of behavioral impairments, including changes in feeding patterns, decreased predator avoidance, and disrupted social interactions can predispose fish to predation, decrease their foraging performance, and affect their reproduction. Moreover, pollution can change the migration behavior of some species and this may disrupt their breeding cycle and cause the population to decrease (Zhang et al., 2025).

Water pollution has far reached ecological consequences on the behavior and health of fish. As an example, fish are very important in terms of nutrient cycle, pests and biodiversity. These important ecosystem services can be disrupted by a decrease in fish population. As an example, predatory fish regulate the number of smaller life, and herbivorous fish can regulate the number of algae, so that the overall balance of the aquatic environment is achieved. In a situation where fish populations are affected by pollution, these ecological processes may be unbalanced leading to harmful algal bloom, species change and even collapse of the ecosystem. Although the negative consequences of water pollution are increasingly proven in relation to aquatic organisms, the longitudinal evaluation of the adverse effect of water pollution on fish behavior and health remain rather limited. Further studies are urgently required to comprehend the extent of these effects, not only as far as the survival of fish but also as to population trends. Moreover, behavioral data assessment would provide a more refined view of the impacts of water pollution in aquatic environments by combining behavioral assessments with conventional water quality assessments (Heath, 2018).

This paper is aimed at explaining the interrelationship of water pollution and fish health and behavior which is complicated. In particular, this research intends to examine the impact of different pollutants on fish on the physiological and behavioral scales with the aim of comprehending the long-term ecological impacts. This paper, by offering an elaborate discussion of the water pollution effects on fish, will help add to the existing literature on environmental pollution and its consequences to aquatic environments. Finally, the results of this study can be used in future conservation and pollution management plans and policies that are designed to safeguard the health and biodiversity of aquatic life.

Types of Water Pollutants Affecting Fish

Heavy Metals

Some most poisonous pollutants among aquatic systems include heavy metals, such as mercury, lead, arsenic, and cadmium. These are non-biodegradable which means that they become concentrated in the environment and in aquatic life especially fish.

- **Mercury:** Mercury is one of the worst heavy metals and it is bioaccumulated in fish. Extended exposure to mercury may have dreadful neurological effects that result in brain damage and behavioral changes. This causes a shift in feeding patterns, reduced predation evasion, and poor mating. Magnification of mercury also involves the increased troic levels and in humans taking mercury-contaminated fish.

- **Cadmium and Lead:** The functioning of the kidneys and liver of fish is interfered with in both cadmium and lead, causing organ damage and a change in the metabolic rates. These metals as well impair the immune system which causes fish to be more vulnerable to diseases.
- **Consequences:** The concentration of heavy metals in fish carries its dangers not just to fish, but to the food chain in general. Being the predators, they are also affected by the pollution of fish and result in ecological imbalances (Jacquin et al., 2020).

Pharmaceuticals and Pesticides

Another major source of water pollution due to pesticides, herbicides and pharmaceuticals include agricultural runoff. These chemicals in most cases find their way into the water bodies through runoffs after rain or irrigation, which influences the quality of water.

- **Pesticides:** Some of the widespread pesticide-use products such as neonicotinoids, organophosphates, and pyrethroids are known to affect the neurological and hormonal functions of fish. When animals are subjected to such chemicals, it may cause changes in their behavior such as less feeding behavior, change in swimming behavior and be exposed to predators.
- **Pharmaceuticals:** Wastewater discharge is increasingly finding its way in rivers and lakes with discharge of pharmaceuticals such as antidepressants, painkillers and antibiotics. Low doses of pharmaceutical contaminated environment among fish lead to behavioral aberrations including altered mating behavior, diminished aggression as well as an impaired predator prey response. In other instances, there can be suppression of immune system that results in increased disease susceptibility in fish. Consequences: Long term population depletion (state of low reproductive performance, poor health, and modulated ecological functions in aquatic systems) could occur as a result of these chemicals (Malik et al., 2020).

Eutrophication and Organic Contaminants

The effects of organic or petroleum hydrocarbons, persistent organic pollutants (POPs), and fertilizers containing nutrients have a major impact on the health of fish.

- **Nutrient Pollution and Eutrophication:** Overuse of farming fertilizers contributes to the drainage of nutrient minerals in the water bodies (Nitrogen and phosphorus). These nutrients result in eutrophy that results in algal blooms. The degradation of the algae reduces the level of oxygen in the water forming hypoxic areas (areas with low oxygen levels), causing suffocation to fish and any other aquatic organism. Hypoxia can cause death or slowed development in fish and impacts their reproduction and survival of fish species.

- **Oil Spills and Hydrocarbons:** These are hydrocarbons such as petroleum soap discharged by oil spills, industrial discharges that contaminate aquatic systems leading to respiratory illnesses, organ damage and death of fish. The hydrocarbons are also known to interfere with the reproductive processes and result in deformed fish offspring.
- **Effects:** Organic contaminants and eutrophication have a feedback loop of deteriorating water quality which further aggravates the health issues experienced by aquatic organisms (Cox et al., 2018).

Table 1. Types of Water Pollutants and Their Effects on Fish Health

Pollutant Type	**Example Pollutants**	**Effects on Fish Health**	**Consequences**
Heavy Metals	Mercury, Cadmium, Lead, Arsenic	Impaired neurological function, liver damage, gill damage, immune suppression	Reduced metabolic function, increased disease susceptibility
Pesticides and Herbicides	Neonicotinoids, Organophosphates, Pyrethroids	Neurological damage, reduced feeding activity, altered reproductive behavior	Decreased reproductive success, altered predator-prey interactions

Pollutant Type	**Example Pollutants**	**Effects on Fish Health**	**Consequences**
Pharmaceuticals	Antidepressants, Painkillers, Antibiotics	Hormonal disruption, altered behavior (e.g., reduced aggression, impaired mating)	Behavioral anomalies, increased vulnerability to diseases
Organic Contaminants	Petroleum hydrocarbons, Persistent Organic Pollutants (POPs), Fertilizers	Respiratory distress, liver damage, hypoxic conditions from eutrophication	Mortality, developmental anomalies, reduced fitness
Nutrient Pollution (Eutrophication)	Nitrogen, Phosphorus from agricultural runoff	Algal blooms, hypoxia (low oxygen), suffocation, stunted growth	Fish kills, disruption of reproduction, population declines

Impacts on Fish Health

Physiological Effects

Aquatic organisms are quite sensitive to environmental variations and when fish are exposed to pollutants; they may have diverse physiological effects.

- **Gill Damage:** Heavy metals, toxins and pollutants may cause damage to the gills of fish making the fish unable to extract oxygen in water. This causes breathing difficulty and fewer survivability rates.
- **Dysfunction of liver:** There are such pollutants as pesticides and metals, which are stored in liver, causing disturbance to the rest of the body to be toxic. This results in liver dysfunction with time and may impact on the metabolism and growth of the fish.

- **Immunosuppression:** Prolonged exposure to the pollutants compromises the immune system leaving the fish susceptible to infections, diseases and parasites. This may cause mass death of fish, which interferes with the local ecologies.
- **Fortune:** The impairments that are born by pollution are imparted on the physiological system of the fish thereby decreasing their lifespan, growth, reproductive capacity which has a resultant impact on fish populations and food chain (Pollock et al., 2007).

Reproductive and Developmental Disturbances

Most divers contaminate marine animals especially endocrine disrupting chemicals (EDCs), which disrupt the fish reproductive system. Change in Sex Ratio, Feminization of male fish as a result of association with chemicals like bisphenol A (BPA) and phthalates or even impaired sexual differentiation. This creates distorted sex ratios thus lowering the overall reproductive success of a fish population.

- **Decreased Fertility:** Heavy metals and pesticides are some of the pollutants that are known to disrupt the formation of eggs and sperm hence reducing fertility rates among fish. This interferes with population recovery and growth. Developmental Anomalies A pollutant has the capability to induce developmental anomaly in fish larvae and embryos such as deformity of the body structure and organs. Such distortions might not allow the survival of those larvae to their adult stages consequently reducing the population further.
- **Consequences:** When reproductive health and development processes are disrupted, any fish population becomes destabilized, which causes losses in the long run (Sharma et al., 2019).

Behavioral Alterations

Neurotoxic Effects

The effects of the pollutants are usually neurotoxic on the fish like heavy metal, pesticides and pharmaceuticals. These neurotoxins disrupt the normal operation of the nervous system and the brain.

- **Cognitive Impairment:** The pollutants may result in cognitive impairment of fish such as memory loss, distorted decision making, and learning impairment. Such shortages impair the foraging, avoidance and navigation capabilities of fish.
- **Altered Social Behavior:** Fish that are exposed to neurotoxic substances might also respond with abnormal social behavior including disrupted group biases or violent behavior. This has an influence on their capacity to create

schools or cooperate in hunting and defense techniques (Atchison et al., 1987).

Altered Activity Patterns

When fish are subjected to pollutants, they tend to change their activity patterns and this may have enormous ecological impacts.

- **Slowed Swimming and Feeding:** Pesticides and heavy metals could lower the level of activity of the fish including the swimming tempo and feeding rate. This lowers their energy consumption resulting to malnutrition and less growth.
- **Disturbed Migration Maps:** There are pollutants that disrupt the fish migration and navigation. This is especially worrisome to the species that depend on long-distance migration during breeding i.e. salmon.
- **Effects:** Fish that is changed in activity patterns would be more susceptible to predation, less successful in reproduction, and their natural distribution in aquatic ecosystems affected (Weis, 2014).

Ecological and Evolutionary Homages

Effects of water pollution on fish health and behavior are far-reaching that individual fish, but on a population and the whole ecosystem.

- **Reduced Fitness:** The pollution causes behavioral and physiological damages, resulting in reduced fitness of fish, where there are fewer fish which survive, reproduce, and transmit their genes. This may in the long run lead to population decreases.
- **Change in Species Composition:** Since some species of fish are more vulnerable to pollutants than others, pollution may lead to species change in aquatic ecosystems. The pollution can select some pollution-tolerant species thus leading to a decrease in biodiversity.
- **Ecosystem Disturbance:** Fish are also important components of an aquatic food web, and their reduction may have cause and effect effects on other organisms; predators, prey and even plants. This may cause the failure of the health status of complete aquatic ecosystems (Kasumyan, 2001).

Strategies of Monitoring and Assessment

It is important to monitor the effects of the pollutants on fish health and behavior to detect the issues and take the corrective action.

Behavioral Biomarkers

Fish behavior may be used as an early warning on the existence of environmental stressor due to pollutants. Pollution can be detected before it may cause major physiological damages by behavioral biomarkers that include alterations in swimming patterns and feeding habits, in social interactions.

- **Methods:** Behavioral analysis: Behavior changes in fish can be determining by behavioral tests, e.g. video tracking, automated monitoring systems. These are non-lethal techniques, which enable a researcher to examine fish in the natural environment, without inflicting damage (Turner et al., 2023).

Integrated Monitoring Systems

When fish behavior is integrated with the conventional measurements of water quality (e.g. oxygen, pH, temperature), this could be a more holistic measure of health in water. Such technologies as remote sensing and sensors based on the Internet of Things (IoT) provide an opportunity to monitor water quality and fish behaviors in real time and use the information to control pollution (Weis et al., 2001).

Formulation and Strategy of mitigation and management

Pollution Source Control

It is possible to have stronger measures on industrial effluents, agricultural discharges, and wastewater treatment, which will greatly decrease the number of adverse pollutants that find their way to the aquatic environments. Use of pesticides, fertilizers and industrial chemicals should be reduced to ensure the health of fish is preserved (Portz et al., 2006).

Habitat Restoration

Wetlands, riparian buffers as well as natural filtration system restoration can be treated to enhance water quality and offer safe fish habitats. Such restorative activities may help diminish the effect of the pollutants and increase the population of fish.

For every policy-related concern, social awareness is necessary including the advocacy of laws and regulations on cognitive dissonance within the community. <|human|>7.3 Public Awareness and Policy Advocacy need social awareness regarding each policy issue, such as the support of cognitive dissonance laws and regulations to the community.

The most important actions towards reducing the effects of pollution to the aquatic life are publicizing how water pollution can affect fish and enforcing stricter environmental policies. More sustainable water management can be achieved by engaging local communities, industries and policy makers in conservation activities (McKenzie et al., 2007).

Conclusion

Water contamination is causing immense impact on the health and behavior of fish and with serious impacts on the aquatic environment. The ecological consequences of the physiological and behavioral disturbances of the pollutants may result in falling population, alteration of species balance, and permanent alterations of the ecological conditions. Just as the strict regulation, restoration of habitats and the populace participation is the way to the causes of pollution to protect fish population and sustain healthy aquatic environments. The effects of pollution can be reduced through combined efforts of monitoring and management to ensure that the water resources are used in a sustainable manner by the future generations.

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Mechanistic Insights into Phosphonium-Mediated Solvent Extraction of Copper, Cadmium, and Zinc

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Abstract

This chapter investigates the solvent extraction behavior of copper (Cu), cadmium (Cd), and zinc (Zn) from aqueous solutions using phosphonium-based ionic liquids as extractants. The extraction efficiency, selectivity, and mechanism are examined under varying conditions including pH, metal ion concentration, and the nature of the phosphonium ion. The study highlights the significant role of phosphonium ionic liquids in enhancing the separation and recovery of these metal ions due to their unique chemical properties, such as high thermal stability, low volatility, and strong metal-binding capabilities. Experimental results demonstrate that phosphonium ions exhibit selective extraction efficiencies for Cu, Cd, and Zn, with Cu showing the highest affinity under optimized conditions. The chapter also discusses the thermodynamics and kinetics of the extraction process, providing valuable insight into the potential industrial applications of phosphonium-based solvent extraction systems in hydrometallurgy and wastewater treatment.

Keywords: Phosphonium ionic liquids; Metal ion separation; Hydrometallurgy; Wastewater treatment; Solvent extraction; Liquid–liquid extraction

Introduction

Solvent extraction, or liquid–liquid extraction, is a well-established method for selectively recovering metal ions from aqueous solutions. It is especially effective for metals such as copper (Cu), cadmium (Cd), and zinc (Zn), given their industrial relevance and environmental impact (Ritcey, 2022). In recent years, phosphonium-based ionic liquids and salts have gained attention as extractants due to their distinctive physicochemical properties (Kumar et al., 2020).

The recovery and separation of valuable metals from aqueous streams play a vital role in hydrometallurgy, environmental protection, and industrial waste management. Among available separation methods, solvent extraction (SX) is one of the most efficient and widely used (Moyer & Singh, 2018). This process transfers metal ions from an aqueous phase into an immiscible organic phase with a suitable extractant, forming metal–extractant complexes that can later be stripped and recovered (Rydberg et al., 2004).

Phosphonium-based ionic liquids and salts, particularly tetraalkylphosphonium ions, have emerged as highly promising extractants. Their advantages include high thermal stability, low volatility, adjustable polarity, and strong affinity for metal ions (Zhang et al., 2021). These properties enable the formation of stable complexes with transition metals, allowing effective separation even in the presence of competing ions (Papaiconomou et al., 2012).

Research has extensively explored their application in extracting Cu^{2+}, Cd^{2+}, and Zn^{2+}. Copper is essential in electrical and construction industries, cadmium—though toxic—is used in batteries, and zinc plays a key role in galvanization and alloys (Habashi, 2017). Efficient recovery of these metals not only conserves natural resources but also reduces environmental risks linked to industrial and electronic waste (Nayl et al., 2020).

This chapter examines the principles, mechanisms, and recent advances in using phosphonium ions for solvent extraction of Cu, Cd, and Zn, with attention to their benefits, extraction performance, and potential applications in hydrometallurgical and environmental fields.

Ingredients / Materials

- Copper (II) sulfate ($CuSO_4$) — as a source of Cu^{2+} ions
- Cadmium (II) nitrate ($Cd(NO_3)_2$) — as a source of Cd^{2+} ions
- Zinc (II) sulfate ($ZnSO_4$) — as a source of Zn^{2+} ions
- Phosphonium salt extractant (e.g. methyltrioctylphosphonium chloride) — the key solvent extraction agent
- Organic solvent (like kerosene, chloroform, or toluene) — to dissolve the phosphonium extractant
- Aqueous phase — distilled or deionized water, with controlled pH
- Buffer solution — to maintain pH during extraction (e.g. acetate buffer)
- Acids and bases (HCl, HNO_3, NaOH) — for pH adjustment
- Separatory funnel — for carrying out solvent extraction
- Beakers, flasks, pipettes — for solution preparation and transfer

- Magnetic stirrer and stirring bars — to mix phases properl
- pH meter
- Atomic Absorption Spectrophotometer (AAS) or Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES) for metal concentration analysis
- Analytical balance — to accurately weigh chemicals

Principal of Solvent Extraction

Solvent extraction involves the transfer of metal ions from an aqueous phase to an organic phase containing an extractant. The efficiency of this process depends on factors such as pH, temperature, metal ion concentration, and the nature of the extractant. The extracted metal ions form neutral or charged complexes with the extractant, which then partition into the organic phase. Solvent extraction is an important separation and purification technique widely used for the recovery of metals from aqueous solutions. This process involves the transfer of metal ions from an aqueous phase into an organic phase containing a suitable extractant. In the context of this study, phosphonium ions are employed as the extractants for selectively separating and recovering Copper (Cu), Cadmium (Cd), and Zinc (Zn) ions.

The extraction process is based on the principle of chemical affinity between the metal ions and the phosphonium ion extractant. Phosphonium salts, typically quaternary phosphonium compounds, possess a high affinity for metal ions due to their ionic and hydrophobic characteristics, making them highly effective in liquid-liquid extraction systems.

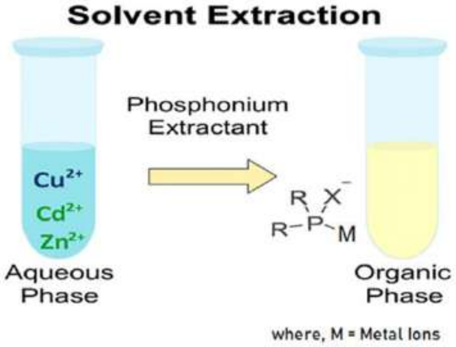

Figure 1: Solvent Extraction of Cu (II), Cd (II) and Zn (II)

During the extraction, the metal ions in the aqueous phase interact with the phosphonium ions in the organic solvent, forming stable, extractable metal-phosphonium complexes. The efficiency and selectivity of this process are influenced by several factors, including:

- pH of the aqueous phase
- Type and concentration of the phosphonium extractant

- Presence of competing ions
- Temperature
- Contact time and phase ratio

By carefully controlling these parameters, it is possible to achieve selective extraction of Cu, Cd, and Zn ions from complex mixtures. The fundamental principle involves the equilibrium distribution of metal ions between the two immiscible phases, guided by the metal's affinity for the extractant and the thermodynamic stability of the formed complexes.

Procedure

Preparation of Aqueous Metal Solutions

- Prepare individual aqueous solutions of Copper (Cu^{2+}), Cadmium (Cd^{2+}), and Zinc (Zn^{2+}) using their respective metal salts (such as $CuSO_4$, $Cd(NO_3)_2$, and $ZnSO_4$).
- Adjust the concentration of each metal ion solution to the desired level (e.g., 0.01 M).

Preparation of Organic Phase

- Dissolve the phosphonium ion-based extractant (such as $[PR_4][A]$) in an organic solvent like toluene or chloroform.
- Maintain the desired concentration of the extractant (e.g., 0.05 M).

Adjustment of pH

- Adjust the pH of the aqueous metal solutions using dilute HCl or NaOH to the targeted value suitable for extraction (typically between pH 2 and pH 6 depending on the metal).

Solvent Extraction Process

- In a separatory funnel, mix equal volumes of the aqueous metal ion solution and the organic phosphonium solution (e.g., 10 mL each).
- Shake the mixture vigorously for a specified time (e.g., 5–10 minutes) to ensure proper phase contact.
- Allow the mixture to stand until clear separation of the two phases occurs.

Phase Separation and Collection

- Carefully separate the organic and aqueous phases.
- Retain both phases for analysis.

Determination of Metal Ion Concentration

- Measure the remaining concentration of metal ions in the aqueous phase using Atomic Absorption Spectroscopy (AAS) or Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES).

- Calculate the extraction efficiency and distribution ratio based on initial and final concentrations.

Repeatability and Optimization

- Repeat the extraction process by varying parameters such as pH, extractant concentration, and contact time to optimize the extraction efficiency for each metal.

Extraction of Copper (Cu)

Copper is widely used in electrical industries and is extracted by solvent extraction from leach liquors derived from ores and secondary sources. Traditionally, hydroxyoximes have been employed, but phosphonium-based ionic liquids have emerged as potential alternatives due to their high selectivity and stability. Solvent extraction, also known as liquid-liquid extraction, is a widely applied separation process for the recovery and purification of metals such as copper (Cu) from aqueous solutions. In this method, an organic solvent containing a suitable extractant is used to selectively separate metal ions from an aqueous phase.

In the case of copper extraction, phosphonium-based ionic liquids or salts have emerged as efficient extractants due to their high selectivity, thermal stability, and tunable properties. Phosphonium ions can form stable complexes with copper ions (Cu^{2+}), facilitating their transfer from the aqueous to the organic phase.

Mechanism of Extraction

Extraction of copper typically involves the formation of a complex between the copper ions and the phosphonium extractant. The general mechanism can be represented as:

$$\mathbf{Cu^{2+}(aq) + 2[R_3P^+X^-]\ (org) \rightleftharpoons [CuX_2(R_3P^+)_2]\ (org)}$$

where, $R_3P^+X^-$ represents the phosphonium ion paired with an anion X^-. (aq) and (org) represent the aqueous and organic phases, respectively.

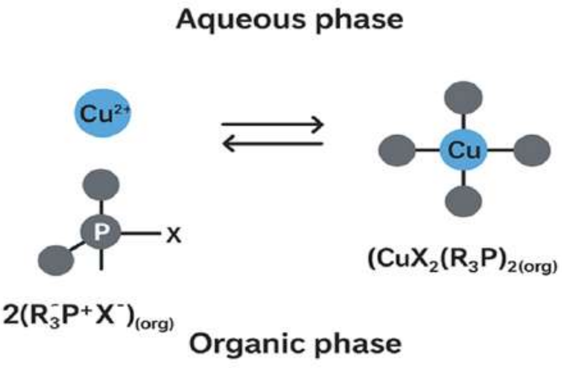

Figure 2: Extraction of Cupper (Cu)

Factors Affecting Copper Extraction

Several factors influence the efficiency of copper extraction using phosphonium ions:

- **pH of the aqueous phase:** Copper extraction generally improves at higher pH values due to enhanced complex formation.
- **Concentration of phosphonium ions:** A higher concentration of the extractant in the organic phase increases the distribution ratio of copper.
- **Temperature:** Higher temperatures may improve extraction kinetics but could affect the stability of the extractant-metal complex.
- **Type of diluent:** The choice of organic solvent can affect the solubility and stability of the phosphonium extractant.
  - ➢ Advantages of Using Phosphonium Ions
  - ➢ High selectivity towards copper ions over other metal ions.
  - ➢ Good thermal and chemical stability.
  - ➢ Ability to tailor the properties of the extractant by modifying the phosphonium structure.

Applications

- The solvent extraction of copper using phosphonium ions is applied in:
- Hydrometallurgical processes for copper recovery from ores, leachates, and industrial effluents (Liu et al., 2010).
- Recycling of copper from electronic waste and other secondary sources (Zhang et al., 2013).
- Recovery from acid mine drainage.
- Processing of electronic waste leachates

Extraction of Cadmium (Cd)

Cadmium, a by-product of zinc metallurgy, is toxic and requires careful handling. Solvent extraction using phosphonium-based extractants provides a method for separating cadmium from aqueous waste streams and industrial effluents.

The extraction of cadmium (Cd) from aqueous solutions using phosphonium-based ionic liquids is an important separation technique in hydrometallurgy and environmental remediation. Phosphonium ions, due to their unique chemical properties, offer selective extraction capabilities, especially for soft metal ions like cadmium.

In this process, cadmium is typically present in an aqueous solution in the form of Cd^{2+} ions. The phosphonium ionic liquid acts as an organic phase containing a counter anion capable of forming a neutral complex with cadmium. This allows for the transfer of cadmium from the aqueous phase into the organic phase.

The extraction mechanism generally follows an ion-exchange or complexation process, which can be represented as:

$$\mathbf{Cd^{2+}(aq) + 2R_3R'P^+A^-(org) \rightleftharpoons (R_3R'P)\ _2CdA_2(org) + 2H^+(aq)}$$

where, $R_3R'P^+$ represents the phosphonium cation, A^- is the counter anion (such as chloride, nitrate, or thiocyanate), and $(R_3R'P)\ _2CdA_2(org)$ is the cadmium complex in the organic phase.

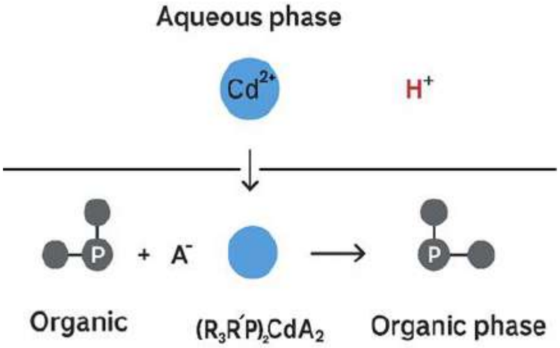

Figure 3: Extraction of Cadmium (Cd)

Key Factors Influencing the Extraction Efficiency Include

- **pH of the Aqueous Phase:** Optimum extraction of Cd generally occurs in a mildly acidic to neutral environment.
- **Type of Phosphonium Ionic Liquid:** The structure of the phosphonium ion and the nature of the anion significantly affect the extraction capacity and selectivity.
- **Temperature:** Increasing temperature may enhance the extraction rate but can also impact the stability of the extracted complex.
- **Phase Ratio:** The ratio of organic to aqueous phase plays a role in determining extraction efficiency and equilibrium.

After extraction, cadmium can be recovered from the organic phase by stripping with an appropriate reagent, often a strong acid or chelating agent, allowing the phosphonium ionic liquid to be recycled for repeated use. This method offers advantages such as high selectivity, low volatility, and reusability of the phosphonium ionic liquid, making it an environmentally friendlier alternative to traditional solvent extraction systems. (Saji and Reddy, 2001; Wei et al., 2014)

Applications

- Treatment of battery recycling waste
- Removal from electroplating wastewaters

Extraction of Zinc (Zn)

Zinc is a critical metal for various industries, especially in galvanizing and alloy production. Solvent extraction using phosphonium-based ionic liquids has been shown to be effective in separating zinc from mixtures containing other base metals. Zinc (Zn) is an important industrial metal used in a variety of applications including galvanization, alloy production, and battery manufacturing. Efficient extraction and separation of zinc from mixed metal solutions is essential for both environmental and economic reasons.

Solvent extraction is a widely used technique for the selective separation of metals from aqueous solutions. In this study, phosphonium-based ionic liquids or phosphonium salts are used as extractants due to their high selectivity, stability, and tunable properties.

Principle of Extraction

The extraction of zinc involves the transfer of Zn^{2+} ions from an aqueous phase into an organic phase containing a phosphonium ion-based extractant. The extraction efficiency depends on factors such as:

- pH of the aqueous solution
- Concentration of the phosphonium extractant
- Temperature
- Contact time

Typically, zinc is extracted from acidic or neutral aqueous media, where the phosphonium extractant forms a complex with Zn^{2+} ions.

Reaction Mechanism

The general extraction reaction can be represented as:

$Zn^{2+}(aq) + 2(R_3P^+X^-)(org) \rightleftharpoons (R_3P)_2ZnX_2(org)$

where, $R_3P^+X^-$ is the phosphonium salt in the organic phase. Zn^{2+} (aqq) is the zinc ion in the aqueous phase. Zn^{2+} ions form a neutral complex with the phosphonium ion pair and are transferred into the organic phase.

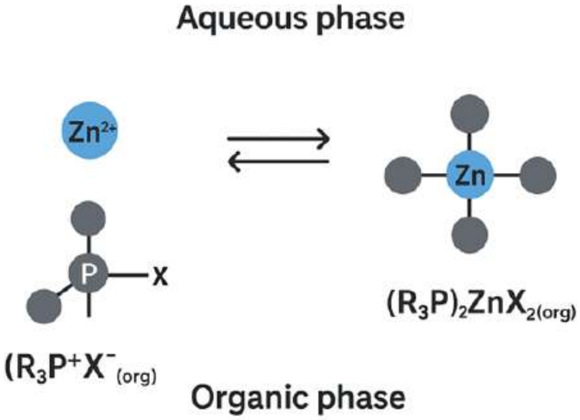

Figure 4: Extraction of Cadmium (Cd)

Factors Affecting Extraction

- **pH:** Optimum extraction occurs at slightly acidic to neutral pH, where zinc exists as Zn^{2+} without significant competition from protons.

- **Extractant Concentration:** Increasing the concentration of phosphonium ions improves the extraction efficiency up to a certain limit.
- **Phase Ratio:** The volume ratio of organic to aqueous phase affects the extent of extraction.
- **Temperature:** Elevated temperatures may enhance the kinetics of extraction but could affect the stability of the complex.
- **Stripping of Zinc:** After extraction, zinc can be stripped from the organic phase by treating it with a suitable stripping agent, typically an acidic solution, regenerating the phosphonium extractant for reuse.

$$\mathbf{Zn^{2+}(aq) + 2R_4P^{+}(org) + 4Cl^{-}(aq) \rightarrow (R_4P)_2ZnCl_4(org)}$$

Applications

- Extraction from zinc plant leachates (Kurniawan et al., 2006).
- Processing of waste pickling liquors (Chen et al., 2016).

Application of Phosphonium Ions

Phosphonium ions, especially those based on tetra alkyl phosphonium structures, exhibit high thermal stability, tunable hydrophobicity, and the ability to form stable complexes with metal ions. Their ionic liquid form enhances phase separation, reduces volatility, and improves extraction efficiencies. Phosphonium ions, a class of organophosphorus compounds containing a positively charged phosphorus atom (typically in the form of R_4P^+), have garnered significant interest in various fields due to their unique chemical and physical properties. Some of the most notable applications include:

- **Solvent Extraction:** Phosphonium-based ionic liquids and salts are widely used as extractants in solvent extraction processes, particularly for the selective separation and recovery of metal ions such as Cu, Cd, and Zn from aqueous solutions. Their high thermal stability, tunable hydrophobicity, and strong complexation abilities make them effective in metal separation technologies.
- **Catalysis:** Phosphonium salts serve as phase-transfer catalysts and ionic liquid media in organic synthesis, enhancing reaction rates and selectivity by facilitating the transfer of reactive species between immiscible phases.
- **Ionic Liquids:** Many phosphonium salts function as ionic liquids, offering applications in electrochemistry, green chemistry, and materials processing. They exhibit excellent thermal and chemical stability, low volatility, and good solvating properties.
- **Electrochemical Applications:** Phosphonium-based compounds are also utilized in electrochemical systems, including batteries and capacitors, due to their ionic conductivity and electrochemical stability.

- **Pharmaceutical and Biomedical Uses:** Some phosphonium compounds have potential in drug delivery systems and antimicrobial formulations, benefiting from their membrane-active properties and ability to transport bioactive ions.
- **Material Science:** Phosphonium ions are employed in the preparation of advanced functional materials, including polymer electrolytes, flame retardants, and nanocomposites, due to their ionic conductivity and structural versatility. These diverse applications highlight the importance of phosphonium ions, particularly in the extraction and separation of metals, which is the focus of this chapter.
- **Separation of Rare and Toxic Metals:** Due to their excellent chelating abilities, phosphonium-based extractants can selectively separate and recover toxic metals such as cadmium from industrial effluents, reducing environmental hazards.

Conclusions

The application of phosphonium ions in solvent extraction processes offers an efficient and environmentally friendly alternative for the recovery of Cu, Cd, and Zn. Their tunable properties, coupled with high selectivity, make them promising extractants for both primary and secondary metal resources.

In this chapter, the solvent extraction behaviour of copper (Cu), cadmium (Cd), and zinc (Zn) using phosphonium ions as extractants was systematically investigated. The study demonstrated that phosphonium-based ionic liquids exhibit strong potential as efficient, selective extractants for these metal ions from aqueous solutions. The extraction efficiency was found to depend significantly on factors such as pH, metal ion concentration, and the nature of the phosphonium ion used. Among the metals studied, copper showed the highest extraction efficiency, followed by cadmium and zinc. The selectivity of phosphonium ions toward Cu over Cd and Zn suggests their practical utility in separating valuable metals from mixed-metal solutions in hydrometallurgical processes and environmental remediation applications.

Overall, this work highlights the advantages of phosphonium ionic liquids, including their tunable properties, chemical stability, and environmental compatibility, providing a promising alternative to conventional solvent extraction systems for the recovery and separation of transition metals.

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Phytochemical Profiling and Ash Analysis of *Majidea zanguebarica* J.Kirk ex Oliv Stem and Leaf Extracts

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Abstract

The present study focuses on the phytochemical profiling, GC–MS analysis and ash value determination of the stem and leaf extracts of *Majidea zanguebarica* (Sapindaceae), an underexplored medicinal plant traditionally used for the treatment of fever, wound infections, and intestinal disorders. Preliminary phytochemical screening of ethanolic and aqueous extracts revealed the presence of bioactive constituents such as alkaloids, flavonoids, saponins, tannins, phenols, and glycosides, which are known to exhibit diverse pharmacological activities. Quantitative estimation indicated a higher concentration of total phenols and flavonoids in ethanolic extracts compared to aqueous extracts, suggesting their potential antioxidant capacity. GC–MS analysis of the leaf and stem extracts identified several important bioactive compounds, including (E)-cinnamaldehyde, phytol, and octadecanoic acid, which have reported antimicrobial and anti-inflammatory properties. Physicochemical parameters such as moisture content, ash value, and extractive value were also evaluated to establish quality control standards for the plant material. The study highlights the medicinal significance of *M. zanguebarica* and supports its potential use as a source of natural therapeutic agents for drug development and formulation.

Keywords: *Majidea zanguebarica*, phytochemical, bioactive, anti-inflammatory, Physicochemical

Introduction

Plants are an abundant source of diverse bioactive compounds that play both direct and indirect roles in the treatment of various human diseases. Since ancient times, human civilizations have explored and utilized different plants and their derivatives to combat a wide range of serious ailments. (Kuldip S Dogra et al., 2015). Medicinal plants have been played an essential role in the development of human culture. Medicinal plants have similar properties as conventional pharmaceutical drugs that human have used throughout history to either cure or lessen symptoms from the illness. Medicinal plants are the backbone of traditional medicines (Deepa and priya 2019).

Phytochemicals are non-nutritive chemical compounds derived from plants that play a significant role in the prevention of human diseases. These include secondary metabolites and antioxidants, which possess important medicinal properties. In some plants, specific phytochemicals serve as a natural defense mechanism, protecting them from insect attacks and grazing animals. Conversely, other phytochemicals contribute to the plant's color, aroma, and flavor, thereby attracting potential consumers (Abhijeet Kasarkar et al., 2018). Phytochemical analysis serves as a key approach in the discovery of new and effective drugs. Plants are among the richest reservoirs of medicinal compounds, providing valuable phytochemical intermediates and chemical entities that form the basis for both traditional medicines and modern synthetic drugs (Hammer et al., 1999).

The Sapindaceae family is well known for its wide range of traditional medicinal applications, including use as a diuretic, stimulant, expectorant, natural surfactant, sedative, vermifuge and in the treatment of stomachache and dermatitis across many parts of the world. Phytochemical investigations of this family have led to the isolation of various secondary metabolites such as saponins, diterpenes, and flavonoids. Several saponins, as well as acyclic sesquiterpene and diterpene oligosides, have been identified as the major secondary metabolites in several Sapindaceae species used in traditional medicine (Perry., 1980).

Majidea zanguebarica is a small tree belonging to the family Sapindaceae, native to East Africa and typically grows up to 5 meters (16 feet) in height. The plant is commonly known as the "Black Pearl Tree" or "Velvet Seed Tree" due to its highly ornamental seeds. It bears dense clusters of small, fragrant greenish-red flowers at the ends of panicles. The fruit is spherical with three lobes, about 3 cm (1.2 inches) long, which split open to reveal a bright red interior containing three smooth, velvety blue-black seeds. Traditionally, various parts of the plant are used to treat fever, wound infections, and intestinal disorders, as the pods and leaves are known to possess antibacterial properties (Aksharadev et al., 2022).

Materials and Methods

Majidea zanguebarica J.Kirk ex Oliv is collected from Rani Anna Govt College campus, Tirunelveli. Mature and healthy plants were collected naturally from the campus after the rainy season (December-January).

Botanical name: *Majidea zanguebarica* J.Kirk ex Oliv

Commen name: Black pearl tree, Magambo tree, Valvet seed tree.

Synonyms: Harpullia zanguebarica

Systematic Position

Kingdom	: Plantae
Division	: Dicotyledons
Class	: Magnoliopsida
Order	: Sapindales
Family	: Sapindaceae
Genus	: *Majidea*
Species	: *zanguebarica*

Methods

Taxonomical and analytical characters were studied in the plant *Majidea zanguebarica* J.Kirk ex Oliv

Macroscopic Observation (Taxonomy)

Fresh plants of *M. zanguebarica* were collected from their natural habitat and brought to the laboratory for taxonomical observation and identification. Morphological characters such as leaf arrangement, venation pattern, flower morphology, fruit and seed characteristics, and stem features were examined carefully. The specimens were studied using a Wexwox Digital Computerized Microscope (Model: BXL-DG 65725). Taxonomical and morphological characters were recorded in standard botanical terms according to relevant floras and taxonomic manuals.

Analytical Studies

For analytical evaluation, the shade-dried leaf and stem powders, along with solvent extracts of the powdered materials, were used. Physico–chemical parameters such as total ash, acid-insoluble ash, water-soluble ash, sulphated ash, moisture content, alcohol-soluble extractive and water-soluble extractive values were determined using standard procedures recommended in the Pharmacopoeia of India (Anonymous, 1996). The extractive values in different solvents were calculated and recorded for comparative evaluation.

A. Determination of Total Ash

Two grams of accurately weighed powdered plant material were placed in a previously ignited and tarred silica dish. The sample was incinerated gradually at a temperature not exceeding dull red heat until it became carbon-free. The dish was cooled and weighed. The total ash content was expressed as a percentage with reference to the shade dried material.

B. Determination of Acid-Insoluble Ash

The total ash obtained above was boiled with 25 mL of dilute hydrochloric acid for five minutes. The insoluble residue was collected on ashless filter paper (Whatman No. 41), washed with hot water, ignited, cooled and weighed. The percentage of acid-insoluble ash was calculated with reference to the shade dried sample.

C. Determination of Water-Soluble Ash

A known weight of the total ash was boiled for five minutes with 25 mL of distilled water, filtered, and the insoluble matter was collected and ignited. The weight difference between total ash and insoluble matter represented the water-soluble ash percentage.

D. Determination of Sulphated Ash

Two grams of powdered plant material were moistened with concentrated sulphuric acid in a nickel crucible and ignited gently. The procedure was repeated until a white residue was obtained. The crucible was cooled and weighed. The percentage of sulphated ash was determined with reference to the shade dried material.

E. Determination of Moisture Content

Two grams of fresh plant material were accurately weighed and dried in a hot-air oven at 105°C. The weight was measured at one-hour intervals until a constant weight was obtained. The loss in weight represented the moisture content.

F. Determination of Alcohol-Soluble Extractive Value

Five grams of the shade dried, powdered sample were macerated with 100 mL of alcohol in a closed flask for 24 hours, with frequent shaking for the first six hours. The mixture was filtered, and 25 mL of the filtrate was evaporated to dryness in a tared dish. The residue was dried at 105°C and weighed. The percentage of alcohol-soluble extractive value was calculated relative to the air-dried sample.

G. Determination of Water-Soluble Extractive Value

Five grams of the powdered plant material were macerated with 100 mL of chloroform water for 24 hours with occasional shaking. The extract was filtered, and 25 mL of the filtrate was evaporated to dryness, dried at 105°C and weighed. The percentage of water-soluble extractive value was calculated with reference to the sample.

H. Determination of Successive Solvent Extractive Values

Ten grams of coarsely powdered plant material were successively extracted in a Soxhlet apparatus using petroleum ether, benzene, chloroform, and methanol until the extract became colourless. After each extraction, the residue was dried below 50°C to remove the remaining solvent. The collected extracts were concentrated by distillation and the yield of each solvent extract was calculated as a percentage of the air-dried sample.

Preliminary Phytochemical Analysis

The powdered plant material was extracted successively using ethanol and distilled water in a Soxhlet apparatus until the extracts became colourless. The extracts were concentrated and subjected to qualitative phytochemical screening following the standard procedures described by Trease and Evans (1989), Harborne (1998), and Brindha et al., (1981).
This analysis aimed to identify the presence of major classes of phytoconstituents such as alkaloids, flavonoids, saponins, tannins, phenolics, steroids, triterpenoids, carbohydrates, catechins, amino acids, and anthraquinones. Observations were recorded as per the standard reaction indications.

Table- 1 Preliminary phytochemical analysis

S.No	Test	Observation	Inference
1	Test solution + a few drops of $CHCl_3$ + 3-4 drops of acetic anhydride and one drop of con.H_2SO_4	Purple colour changing to blue or green	Presence of steroids
2	Test solution + piece of tin + 3 drops of thionyl chloride	Violet or purple colour	Presence of triterpenoids
3	Test solution + 2 ml of Fehling's reagent + 3 ml of H_2O and boil.	Red orange colour	Presence of reducing sugars
4	Test solution + very small quantity of anthrone + few drops of con.H_2SO_4	Green to purple colour	Presence of sugars
5	Test solution taken with (2N) HCl. Aqueous layer formed decanted and to which are added one or two drop of Mayer's reagent	White turbidity or precipitate	Presence of alkaloids
6	Test solution in alcohol + one drop of neutral ferric chloride	Intense colour	Presence of phenolic compounds

7	Test solution in alcohol + a bit of magnesium and one drop of con.HCl and heat	Red and orange	Presence of flavonoids
8	Test solution in alcohol + Ehlrich reagent and a few drops of con.HCl	Pink colour	Presence of catechins
9	Test solution + H_2O and shake	Foamy lather	Presence of saponins
10	Test solution + H_2O + lead acetate	White precipitate	Presence of tannins
11	Test solution + magnesium acetate solution	Pink colour	Presence of anthroquinones
12	Test solution + 1% Ninhydrin reagent	Blue or violet colour	Presence of aminoacids

Quantitative Estimation of Phytochemicals

Quantitative estimation was carried out to determine the total concentration of selected phytochemical groups such as flavonoids, tannins, carbohydrates, amino acids, proteins, lipids, phenolics, and pigments.

A. Estimation of Total Flavonoids

Flavonoid content was determined according to the method of Boham and Kocipal-Abyazan (1974). Ten grams of powdered plant sample were extracted with 80% methanol, filtered and evaporated to dryness. The final residue weight represented the total flavonoid content.

B. Estimation of Tannins (Burade et al., 2005)

Tannins were quantified by the Folin-Denis method based on the reduction of phosphotungsto–molybdic acid in an alkaline medium to a blue complex, with absorbance measured at 700 nm.

C. Estimation of Carbohydrates (Yemm and Willis, 1954)

Carbohydrates were hydrolyzed and reacted with anthrone reagent to form a green chromogen measurable at 630 nm. Glucose was used as the standard.

D. Estimation of Amino Acids (Moore and Stein, 1948)

Free amino acids were estimated using the ninhydrin method, forming a purple complex measured at 550 nm. Results were expressed as glycine equivalents per gram of dry weight.

E. Estimation of Lipids (Bligh and Dyer, 1959)

Lipids were extracted using a chloroform: methanol (2:1) solvent system and quantified gravimetrically after evaporation of the solvent.

F. Estimation of Protein (Lowry et al., 1951)

Protein content was determined using the Folin–Ciocalteu reagent, with absorbance read at 650 nm against a BSA standard curve.

G. Estimation of Phenolic Compounds (Bray and Thorpe, 1954)

Total phenolics were quantified by the Folin–Ciocalteu method, forming a blue complex measurable at 630 nm.

H. Estimation of Chlorophyll and Carotenoids (Arnon, 1949)

Pigments were extracted in 80% acetone, and the absorbance values were measured at 663, 645, and 480 nm to calculate chlorophyll and carotenoid concentrations.

Gas Chromatography–Mass Spectrometry (GC–MS) Analysis

Sample Preparation

Mature and healthy plants were collected, washed and shade-dried for two weeks. The dried samples (leaf, stem, and root) were powdered and subjected to Soxhlet extraction using ethanol. About 60 g of each sample was refluxed with 250 mL of solvent for five hours. The extracts were concentrated and stored for GC–MS analysis.

Instrumental Conditions

GC–MS analysis was performed using a Shimadzu GC–MS–QP 2010 system equipped with a DB1 capillary column (30 m × 0.25 mm i.d.). Helium was used as the carrier gas at a flow rate of 0.7 mL/min. The column temperature was programmed from $70^{\circ C}$ (held for 5 min) to $280^{\circ C}$ at variable ramp rates. Injector and detector temperatures were set at 280°C and 290°C, respectively. One microlitre of the extract was injected in split mode (ratio 3:1). The ionization voltage was 70 eV, and mass spectra were recorded in the 30–600 amu range.

Compound Identification

The compounds were identified by comparing their mass spectra and retention indices with those from the NIST ’98 and Wiley MS libraries, as well as data available in the literature. The identity of each compound was confirmed based on its unique mass fragmentation pattern.

Results and Discussion

Phytochemical Screening

Active components of different parts of *M. zanguebarica* were extracted and analyzed qualitatively and quantitatively. The plant extract contained several active components and secondary metabolites that play an important role in its pharmacological potential. Since different phytochemicals show variable solubility in solvents, the extraction was performed using solvents of different polarities ethanol and distilled water.

The phytochemical screening of both stem and leaf extracts revealed the presence of alkaloids, flavonoids, tannins, saponins, terpenoids, and phenolic compounds in varying concentrations. The ethanolic extract showed a higher intensity of secondary metabolites compared to the aqueous extract, indicating that ethanol effectively solubilizes most bioactive components. These compounds are known for their antioxidant, antimicrobial, and anti-inflammatory activities, which support the traditional medicinal uses of *Majidea zanguebarica*. Similar findings were reported by AK Choudhury et al., (2017), who observed that solvent polarity significantly influences the extraction efficiency of phytoconstituents from medicinal plants.

Table- 2 Preliminary phytochemical analysis of stem and leaf of Majidea zanguebarica.

Solvent	**Plant part**	Alkaloids	**carbohydrates**	**Phenol**	**Saponin**	**Flavonoids**	**Protein**	**Amino acid**	**Catechins**	**Coumarin**	**Quinone**	**Tannin**
Ethanol	**Stem**	-	+	+	+	+	+	_	+	+	+	-
	Leaf	-	-	+	-	+	-	_	-	+	+	-
Distilled water	**Stem**	-	-	#	+	#	-	-	+	#	_	-
	Leaf	-	+	-	+	+	-	-	+	-	_	-

(+)-present, (#)-slightly present, (-)-Absent

The diversity of phytochemicals found in *M. zanguebarica* reflects the plant's adaptability and defence mechanism against environmental stress. These compounds together play an important role in the plant's pharmacological and therapeutic value, making it a potential source for the development of novel herbal formulations.

Quantitative Estimation of Phytoconstituents

Quantitative estimation was carried out to determine the concentration of major phytochemical groups in both stem and leaf extracts of *M. zanguebarica*. The leaf extract exhibited a higher amount of phenols, flavonoids and tannins compared to the stem, confirming its strong antioxidant potential. Alkaloids and saponins were moderately present in both parts. These findings indicate that the leaf may serve as a potent source of bioactive compounds for pharmacological and cosmetic applications.

The results correlate with studies on other medicinal plants, where higher concentrations of secondary metabolites were observed in the leaf portions due to enhanced metabolic activity and sunlight exposure (Krishnaiah et al., 2009).

Quantitative phytochemical analysis of Majidea zanguebarica

S.NO	**Estimation**	***Majidea zanguebarica***	
		Stem	**Leaf**
1.	**Carbohydrates (mg/g/dry wt.)**	**4.41**	**5.22**
2.	**Proteins (mg/g/dry wt.)**	**0.81**	**0.72**
3.	**Amino acids (mg/g/dry wt.)**	**0.82**	**0.21**
4.	**Phenols (mg/g/dry wt.)**	**1.48**	**1.72**
5.	**Tannins(mgkg-1)**	**0.89**	**0.61**
6.	**Flavonoids(mgkg-1)**	**0.42**	**1.60**
7.	**Chlorophyll A (mg/g/dry wt.)**	**0.31**	**1.01**
8.	**Chlorophyll B (mg/g/dry wt.)**	**0.22**	**0.07**
9.	**Carotenoids (moles/g/dry wt.)**	**0.40**	**1.73**

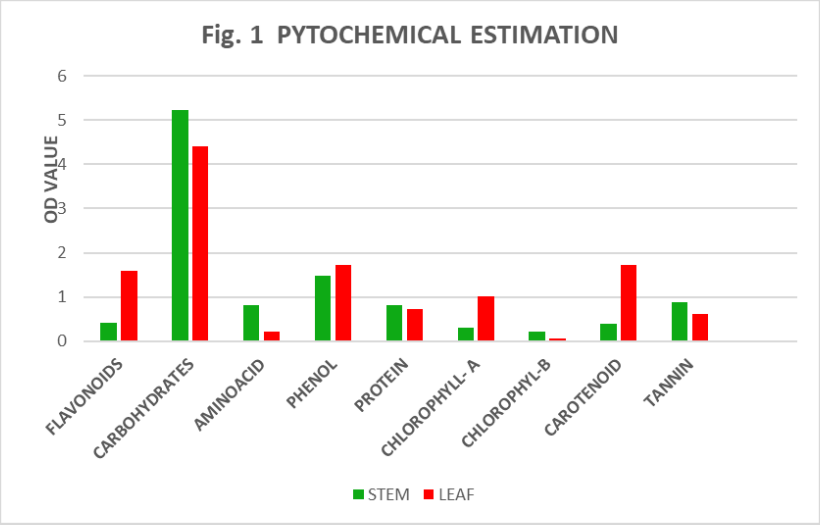


Fig. 1 PYTOCHEMICAL ESTIMATION

The quantitative estimation of phytoconstituents highlights that *M. zanguebarica* is a rich source of natural compounds with significant biological importance. These bioactive molecules may act synergistically to produce antioxidant, antimicrobial, and anti-inflammatory effects.

Physicochemical Analysis

The physicochemical parameters Analysis of the stem and leaf powders of *M. zanguebarica* were analyzed to determine ash values, extractive values, and moisture content. These parameters serve as essential diagnostic tools for the standardization and quality control of crude drugs.

The ash analysis revealed that the total ash content was higher in the stem (11.4%) than in the leaf (6.9%). The acid-insoluble ash (4.58%) was also greater than the water-soluble ash (3.10%) in the stem, suggesting the presence of siliceous matter. The sulphated ash value was 14.5% for the stem and 12.7% for the leaf. The moisture content was comparatively higher in the leaf (9.3%) than in the stem (1.35%), indicating a higher tendency for microbial growth in leaf powders if not properly dried.

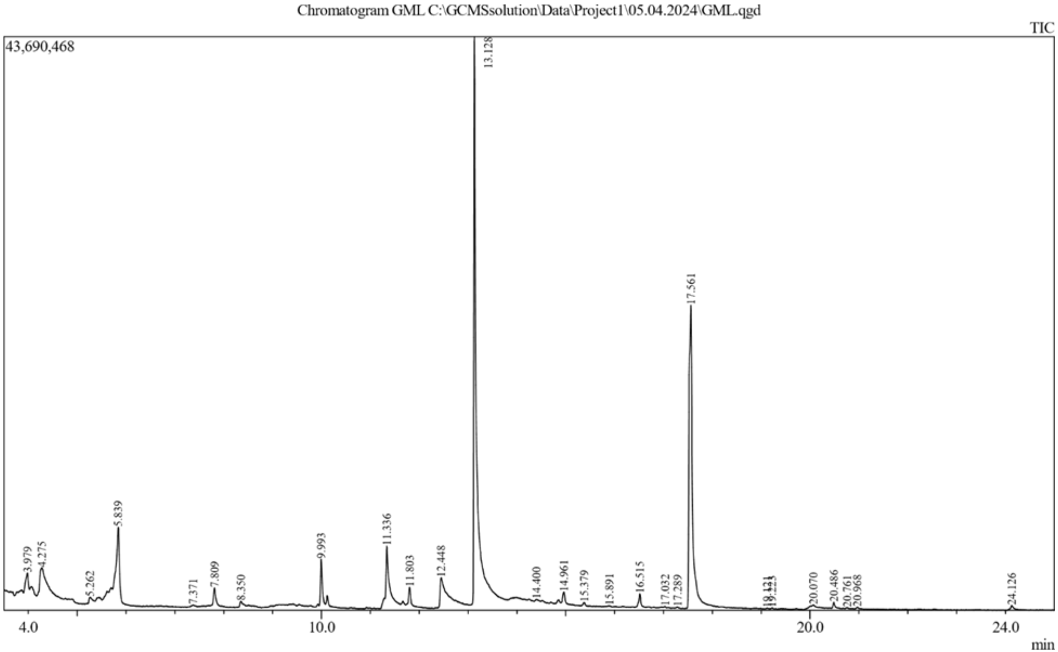
The water-soluble extractive value was found to be 5.1% in the stem and 11.5% in the leaf, while the alcohol-soluble extractive value was 5.6% in the stem and 4.5% in the leaf. These results suggest that polar compounds are more abundant in the leaf extract.

Physico-chemical analysis of *Majidea zanguebarica*

S.NO	TEST	*MAJIDEA ZANGUEBARICA*	
		STEM %	**LEAF %**
1.	**Total ash**	**11.4**	**6.9**
2.	**Water soluble ash**	**3.10**	**2.58**
3.	**Acid insoluble ash**	**4.58**	**4.03**
4.	**Sulphated ash**	**14.5**	**12.7**
5.	**Moisture content**	**1.35**	**9.3**
6.	**Water soluble extractive value**	**5.1**	**11.5**
7.	**Alchocol soluble extractive value**	**5.6**	**4.5**

These parameters provide useful data for standardization, quality control, and storage stability of the plant material, ensuring its suitability for further pharmacological and industrial studies.

Fig-2 GC-MS Analysis in Ethanol Extract of Leaf (M.Zanguebarica)



Peak #	*R.Time*	*Area*	*Area %*	*Height*	*Height %*	*Name*
1	*3.979*	*9342764*	*2.27*	*1581931*	*1.70*	*3-Hexanol, 3-methyl-*

2	4.275	17757288	4.31	2064160	2.22	Dimethyl Sulfoxide
3	5.262	2925378	0.71	425740	0.46	Butanoic acid, 2-hydroxy-2-methyl-, methyl ester
4	5.839	33704812	8.18	5679724	6.10	Pyrrolidine-2,4-dione
5	7.371	589660	0.14	135384	0.15	Tetraethyl silicate
6	7.809	4043995	0.98	1317891	1.41	2,2-Dimethylcyclopropancarboxylic acid,cyanomethyl ester
7	8.350	1644415	0.40	417227	0.45	2-Butenamide, N-(aminocarbonyl)-2-ethyl-, (Z)-
8	9.993	10764105	2.61	3488168	3.74	Linalool
9	11.336	23186447	5.63	4636762	4.98	Benzoic acid, ethyl ester
10	11.803	3787166	0.92	1309668	1.41	Dodecane
11	12.448	15963477	3.87	2144578	2.30	3-Phenylpropanol
12	13.128	165643229	40.19	43221593	46.39	Cinnamaldehyde, (E)-
13	14.400	830081	0.20	139259	0.15	Phenol, 2-methoxy-4-(2-propenyl)-, acetate
14		3974013	0.96	905369	0.97	Tetradecane

	14.961					
15	15.379	525839	0.13	201238	0.22	Caryophyllene
16	15.891	43099	0.01	34561	0.04	9-Oxabicyclo [3.3.1] nona-2,6-diene
17	16.515	2871766	0.70	997645	1.07	2,4-Di-tert-butylphenol
18	17.032	145562	0.04	66965	0.07	Octane, 2-methyl-
19	17.289	245512	0.06	90197	0.10	Hexadecane, 2-methyl-
20	17.561	109541531	26.58	22994537	24.68	Diethyl Phthalate
21	19.121	149736	0.04	62880	0.07	2-(4'-Hydroxyphenyl)-2-(4'-methoxyphenyl) propane
22	19.223	157265	0.04	75826	0.08	3-Methyl-4-(phenylthio)-2-prop-2-enyl-2,5-dihydrothiophene 1,1-dioxide
23	20.070	1417483	0.34	215619	0.23	Tetradecane, 1-chloro-

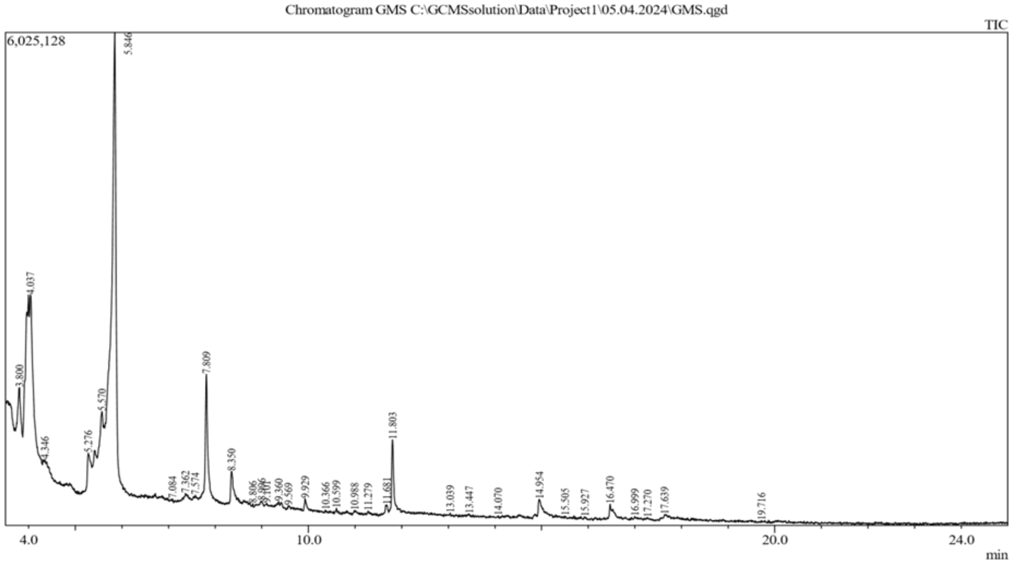
The GC–MS chromatogram of the ethanol extract of *M. zanguebarica* leaf revealed a total of 23 peaks (Table X). The major compounds identified included (E)-cinnamaldehyde (RT 13.128 min; 40.19%), diethyl phthalate (RT 17.561 min; 26.58%), and pyrrolidine-2,4-dione (RT 5.839 min; 8.18%). Other notable constituents were linalool (2.61%), benzoic acid ethyl ester (5.63%), and 3-

phenylpropanol (3.87%).

The presence of (E)-cinnamaldehyde is particularly significant as this compound is well-documented for its antimicrobial, antioxidant, and anti-inflammatory properties (Guo et al., 2024). Similarly, the identification of pyrrolidine-2,4-dione—a compound belonging to the pyrrolidine scaffold family—indicates potential pharmacological relevance, since pyrrolidine derivatives are known to exhibit antibacterial, antiviral, and anticancer activities (Poyraz et al., 2023).

Overall, the leaf extract demonstrated a diverse chemical profile containing both aromatic and heterocyclic bioactives, supporting the plant's traditional medicinal applications. These findings justify further analytical work to isolate, purify, and characterize the major bioactive constituents through advanced chromatographic and spectroscopic techniques.

Fig-3 GC-MS Analysis in Ethanol Extract of Stem (M. Zanguebarica)



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Name
1	3.800	2079847	3.24	553191	4.50	2,2,4-Trimethyl-3-pentanol
2	4.037	17178778	26.78	1800145	14.63	3-Hexanol, 3-methyl-
3	4.346	56072	0.09	47962	0.39	3-Octyn-1-ol

4	5.276	1233111	1.92	342620	2.78	2-Methylbutane-1,4-diol, 3-(1-ethoxyethoxy)-
5	5.570	912285	1.42	297203	2.42	Pyrrolidine-2,4-dione
6	5.846	28803393	44.90	5186581	42.15	Pyrrolidine-2,4-dione
7	7.084	-94	-0.00	20919	0.17	4-Methylfurazan-3-carboxylic acid
8	7.362	228569	0.36	65672	0.53	Tetraethyl silicate
9	7.574	203352	0.32	55212	0.45	Decane, 3,4-dimethyl-
10	7.809	5123003	7.99	1495801	12.16	4-Ethyl-5-hydroxy-3,5-dimethylfuran-2-one
11	8.350	1461201	2.28	377394	3.07	1-(2-Ethylcrotonoyl) urea
12	8.806	31586	0.05	35974	0.29	4,5-Dimethoxy-6-nitropyridin-2-ol
13	8.996	164517	0.26	55122	0.45	2,4,6-Octatrienal
14	9.101	27172	0.04	25877	0.21	5-Allyl-6-methyl-2-phenyl-5,6-dihydro-4H-oxazolo[4,5-c] pyridin-7-one
15	9.360	264927	0.41	58040	0.47	3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene
16	9.569	64556	0.10	31353	0.25	4-Piperidinol, 4-ethynyl-1-methyl-
17	9.929	386798	0.60	138747	1.13	3-Buten-1-ol, TMS derivative

18	10.366	40688	0.06	29181	0.24	3-(Aminomethyl)-1-ethylpyrazol-4-amine
19	10.599	86053	0.13	51535	0.42	Cyclopentasiloxane, decamethyl-
20	10.988	86251	0.13	33909	0.28	Nonane, 4,5-dimethyl-
21	11.279	45743	0.07	33067	0.27	Carbonic acid, di(decyl) ester
22	11.681	286554	0.45	87550	0.71	1-Undecene
23	11.803	2494065	3.89	863154	7.02	Dodecane

Similarly, the GC–MS chromatogram of the ethanol extract of the *M. zanguebarica* stem displayed 23 peaks. The predominant compounds were pyrrolidine-2,4-dione (RT 5.846 min; 44.90%), 3-hexanol, 3-methyl (RT 4.037 min; 26.78%), and 4-ethyl-5-hydroxy-3,5-dimethylfuran-2-one (RT 7.809 min; 7.99%). Other minor compounds such as dodecane (3.89%), 1-undecene, and various decane derivatives were also detected.

The recurring detection of pyrrolidine-2,4-dione in both leaf and stem extracts reinforces its significance as a potentially active compound, consistent with the known pharmacological versatility of pyrrolidine-based molecules (Poyraz et al., 2023). The presence of aliphatic alcohols, furanones, and hydrocarbons further suggests that the stem extract may contain compounds contributing to antimicrobial, antioxidant, and allelopathic activities. Previous reports have demonstrated that the hexane bark extract of M. zanguebarica exhibited significant antidermatophytic activity, indicating its potential for use in the development of novel antifungal drugs (Shyamala gowri Shanmugasundaram., 2020). Moreover, the methanolic flower extract has shown cytotoxic effects against cervical cancer cells, confirming the plant's anticancer potential (Aksaradevi et al., 2022). These findings support the traditional and ethnomedicinal uses of the species in treating various ailments.

The test plant showed both leaf and stem extracts of Majidea zanguebarica exhibit a rich diversity of bioactive secondary metabolites, validating its traditional therapeutic use. The GC–MS results provide a chemical basis for its pharmacological potential and highlight the need for bioassay-guided fractionation and in vitro/in vivo testing to confirm biological activities

Summary and Conclusion

The present study focused on the phytochemical screening and GC–MS analysis of the leaf and stem extracts of M. zanguebarica using ethanol and distilled water as solvents of differing polarity. The extracts revealed the presence of several bioactive phytoconstituents, including alkaloids, flavonoids, tannins, phenolics, saponins, steroids, glycosides, and terpenoids, which are responsible for a wide range of pharmacological activities such as antioxidant, antimicrobial, and anti-inflammatory effects.

The present investigation confirmed that the ethanol extracts of M. zanguebarica contain valuable phytochemicals such as steroids, tannins, and cardiac glycosides, validating their medicinal importance. Based on these findings, it can be concluded that Majidea zanguebarica is a promising medicinal plant with broad-spectrum pharmacological significance. The leaf and stem extracts may serve as rich sources of antioxidant and antimicrobial agents, making them useful in drug formulation and development. Overall, the study provides scientific evidence supporting the traditional uses of M. zanguebarica and highlights its potential for pharmaceutical, nutraceutical, and biotechnological applications.

Future work involving HPTLC profiling, antioxidant assays, and antimicrobial studies will further elucidate the plant's bioactive components and mechanisms of action. To date, no clinical trials have been reported, suggesting that the plant remains an underexplored source of potential therapeutic agents. However, further studies are required for the isolation, purification, and structural characterization of the individual active compounds responsible for these effects.

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Plant Bio-indicators of Air, Soil, and Water pollution: A Critical Review

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Abstract

Environmental pollution caused by urbanization, agricultural and industrialization poses significant threats to ecosystem health. The plants serve as effective bioindicators, providing a valuable insight into the type, intensity and distribution of pollutants across diverse habitats. This review synthesizes research from 2020 to 2025 on vascular plants, bryophytes, lichens and mosses as bioindicators of air, water and soil pollution. Each species demonstrating distinct morphological, physiological, biochemical, or genotoxic responses. Mechanisms such as phenolic accumulation, chlorophyll reduction, heavy metal bioaccumulation and micronucleus formation shows their diagnostic potential. Sensitive species such as lichens (*Plantago coronopus*) provide early warning signals, while tolerant hyperaccumulators species such as *Nuphar lutea, Alcea rosea* shows phytoremediation. The comparative studies reveals that the deciduous plants respond more rapidly to pollution than conifers. Further the scope of plant-based monitoring system enhanced by emerging approaches, including biosensors, electrochemical assays and remote sensing. Overall, the traditional plant bioindicators with modern analytical tools provides a cost-effective, reliable and sustainable strategy for environmental assessment and ecosystem protection.

Keywords: Bioindicators, genotoxic, bioaccumulation, biosensors, electrochemcal, pollution

Introduction

In past few decades, due to various human activities, the release of heavy metals and industrial pollutants has led to widespread environmental degradation, affecting the biosphere along with soil and water system (7). The total energy output from human-induced sources far exceeds that of natural sources (8,31). Industrial technologies often have undesirable consequences on the environment due to gaseous emissions and untreated wastewater containing hazardous compounds. As a result, air pollution and soil contamination have emerged as major threats to plant survival in industrial vicinities and are recognized as potential causes of land degradation (15). Bioindicators play a crucial role in this context, as they can detect signals across multiple temporal and spatial scales, providing a consolidated assessment of ecosystem stresses. However, since bioindicators themselves are affected by these stresses, they are often species that show tolerance to certain stress factors (20). Understanding the physiological mechanisms such as the uptake and accumulation of pollutants in their tissues provide valuable insights into how these stresses impact bioindicators. This knowledge helps in designing effective bioindicators for future monitoring. An ideal bioindicator should exhibit a measurable response to environmental stress, and if the fate of pollutants within its body is known, its better understood (16). The toxic effects of metals on plants, for instance, may manifest as nutrient deficiencies, impaired water transport, reduced photosynthesis, or various morphological, physiological, and biochemical disturbance (13). Identifying plant traits that reliably indicate pollution requires specialized methodologies and the application of modern analytical tools (30,34). Despite this, relatively few studies have examined plant responses specifically to atmospheric air pollution. Research in this direction is increasing, with plants being used both to assess the impact of major anthropogenic systems on air quality and to monitor the environmental state of densely populated or industrialized regions (24,19).

Land, water and air are vital natural resources that transcend political boundaries and represent a shared concern for all of humanity (9). Within this context, specific plant species have proven to be valuable indicators of wetland ecosystem health. Beyond their bioindicator role, many of these plants are also recognized for their capacity to reduce pollutants through phytoremediation (a process in which contaminants are absorbed, accumulated and assimilated into plant tissues). This ability is driven by distinct physiological mechanisms, particularly the uptake of pollutants through roots and shoots (14). Building on existing literature, the present study aims to provide an overview of plant bioindicators in wetlands, focusing on their dual role in detecting and mitigating environmental stressors such as heavy metals, excess nutrients, urban runoff, wastewater, and water quality parameters associated with pollution (12). Aquatic plants not only provide critical insights into the condition of aquatic environments and serve as reliable indicators for biological monitoring of pollution, but they also play a vital role in removing contaminants such as dyes, heavy metals, hydrocarbons, pharmaceuticals, and pesticides from water (6). Many aquatic species are recognized as effective phytoremediators, capable of bioaccumulating toxins in their tissues and thereby contributing significantly to the reduction of aquatic pollution (4). Similarly, air pollution remains a major global concern due to its detrimental impacts on both living organisms and non-living components of the environment. To classify an area as polluted, comprehensive environmental assessments, either bottom-up or top-down are essential (25). Air pollution is defined as the presence of harmful substances in the atmosphere, occurring in the form of solid particles, liquid droplets, or gases, all of which can pose serious risks to human health and ecological systems (22).

Materials and method

The present review was based on a comprehensive survey of published research papers from 2020 to 2025, focusing on the role of vascular plants, bryophytes, lichens, and mosses as bioindicator of environmental pollution (land, air and water) (11). The relevant peer-reviewed articles, books, and reports were collected using electronic databases includes Google Scholar. The following keywords and their combinations were used: Plant bioindicators, phytoremediation, air pollution, heavy metals, urban vegetation, lichen bioindicators, moss bioindicators, and industrial pollution (3,5,17,).

From the reviewed literature, more than 35 species were identified as environmental bioindicator (land, air and water). From these species, Woody ornamentals (*Bougainvillea glabra, Pinus sylvestris*, deciduous plants) act as effective indicators of urban and industrial air pollution, showing that morphological changes, fluctuating asymmetry, or biochemical responses eg., high phenolics, chlorophyll reduction. Leguminous grasses, Nuphar lutea, *Glycine max, Alcea rosea, and Plantago spp*., accumulate heavy metals and exhibit oxidative stress, altered photosynthetic efficiency, and tissue level accumulation, marking them as suitable accumulators and phytoremediators. Annual vs. perennial species from cement polluted zones (*Plantago coronopus vs. Artemisia herba-alba*) reveal differences in sensitivity and tolerance with annuals disappearing under stress and perennials adapting. Cryptogames remain highly sensitive indicators of gaseous pollutants (SO2, NOX, CO, dust) and heavy metals, reflecting changes in species richness, abundance, and morphology. Tradescantia pallida serve as a genotoxicity bioindicator detecting airborne mutagens through micronucleus formation. Wild or ruderal plants a halophyte (*Spartina alterrniflora, Carpobrotus acinaciformis*) demonstrate the potential to indicate and bioaccumulation.

Result and Discussion

Table-1: Plant Species that Serves as Bioindicators

Species	**Pollutant**	**Habitat**	**Bioindicator Type**	**Response/ Mechanism**	**Reference**
Bougainvillea glabra	Particulate matter, heavy metals in air and soil (Fe,Cu,Cd,Zn,Mn,Pb,Ni,Cr,Co)	Industrial zones	Biochemical and Morphological Indicator	High level of pheonolics and flavonoids in leaves causes morphological changes	3
	Dust/Airborne particles	Industrial zones	Physiological Indicator	Dust deposition in the leaf surface reduces the chlorophyll synthesis	
	Air pollution (TSP, PM_{10}, NO, NO_2, NOx, SO_2, CO, CO2)	Industrial zones	Morphological Indicator	Leaf morphology, growth and productivity changes	
Leguminous grass	Zn,Cd,Cu,Fe,Ni, Mn	Agricultural soil	Accumulator/Phytoremediator	Heavy metal content from the stemming phase to flowering	17
Annual species (*Plantago coronopus, Plantago Arabica, Erodium retusa*)	Cement dust	Control site	Sensitive species indicator	Absent in polluted area	5
Perennial species (*Arthrocnemum armatus, Artemisia herba alba, Helianthemum kahiricum*)	Cement dust	Control site	Sensitive species indicator	Absent in pollutant area	
A.serratuloides, L.spartum, G.decander	Cement dust and Cr, Co, Zn, Pb	Polluted zones	Accumulator/Tolerant Indicator	For sink-trap species and offer their possible use in phytoremediation perspectives in a context of sustainable development	
Nuphar lutea leaves	Cd, Cr, Fe, Ni, Zn (Sediments)	Urban and Agricultural areas	Sediment pollution indicator	High metal levels in sediments, reflected in leaf concentration.	21

	Cr, Fe, K	Urban area	Metal specific indicator	High levels of metal contet in leaves indicate urban pollution	
	Cd	Agricultural areas	Metal specific indicator	Highest Cd conc. in leaves (fertilizers and pesticides)	
	Co, Mn, Ni, Pb, Zn	Forest areas	Low pollution reference	Low level of metal content in leaves indicate minimal human impact	
Wild and ruderal plants	PAHs, other contaminants	Urban and Rural	Accumulative, Comparative	Absorb pollutants from air, irrigation water and soil	32
Glycine max	La and Pb	Argicultural/ Urban, rainwater,soil	Biomarker, Electrochemical biosensor	High metal exposure causes oxidative stress, endocytosis, membrane damage and growth inhibition	33
	La+Pb	Industrial areas	Damage assessment indicator	Combined La+Pb stress at high levels is additive	
Vascular plants and Bryophytes	Industrial pollutants	Industrial zone	Phytoindicators, hyperaccumulators	Plants show structural plasticity and resistance to pollution	2
Pinus sylvestris L.	Air pollutant (urban, traffic, industrial)	All functional zones of Dubna	Coniferous bioindicator	Used to detect zoning of air quality, Shows stress due to air and possibly groundwater contamination	28
Deciduous woody and herbaceous plants	Air pollutant (traffic, industrial)	All functional zones of Dubna	Leaf fluctuating asymmetry	Sensitive to habitat changes caused by motor transport and industrial emissions	
Pinus sylvestris L. and deciduous spp.	Urban area pollutant	Urban landscape in Dubna	Comparative phytoindicator system	Deciduous plants reflect current pollution levels due to faster response and seasonal growth	

Lolium multiflorum var. ponto, Rumex acetosa L., Amaranthus retroflexus L., Plantago lanceolata L., Alcea rosea L., Lolium multiflorum L. var. Ponto	Cu, Zn, Cd, Pb	Urban soils, Poznan city	Reduction of chlorophyll content and relative water content, but in efficiency of photosynthesis parameters: net photosynthesis rate, intercellular CO2 concentration and stomatal conductance, we noted increased values, which proved the relatively good condition of the plants.	High level of Cd and Zn roots and leaves of *Alcea rosea* L.and Plantago *lanceolata* L. H_2O_2 level increases in roots and leaves of all species	10
Foliose - *Phaeophyscia orbicularis, Xanthoria parietina, Parmelia sulcata, Hypogymnia physodes* Crustose – *Lecanora conizaeoides* Fruticose – *Evernia prunastri, Ramalina farinacea*	Sulfur Dioxide, Nitrogen Dioxide, Dust, Carbon monoxide	Poltava and Kharkiv (central part, industrial areas, sleeping areas, park areas and green spaces)	Lichen indicator species	Shows strong correlation with pollution levels, Sensitive to air quality	26
Spartina alterniflora, Carpobrotus acinaciformis	Trace elements and Beach litter (mainly plastics)	Terrestrial	Bioaccumulation of metals	Demonstrating its utility in assessing beach pollution	27
Lichens	SO_2, NO_X, heavy metals	Trees, rocks, buildings	Natural bioindicator	Changes in species diversity, abundance, and morphology due to pollutant sensitivity	
Mosses	Heavy metals, nitrogen compounds	Moist, shaded surfaces	Natural bioindicator	Absorption and retention of airborne pollutants in tissue	

Tradescantia pallida	Airborne mutagens/genotoxins	Gardens, urban green spaces	Natural bioindicator	Micronucleus formation in plant cells as an indicator of genotoxicity	

By using Systematic Literature Review, research on plant bioindicators has expanded to cover a wide taxonomic range, including vascular plants, bryophytes, lichens, mosses, grasses, and woody trees. These taxa are distributed across diverse habitats includes industrial zone, agricultural fields, forest areas, urban landscapes, and coastal environments shows the broad applicability of plant bioindicators in different ecological contexts (Table-1).

Pollutant Specificity and Detection Mechanism

The reviewed studies reveal a strong focus on heavy metals (Cd, Pb, Zn, Cu, Ni, Mn, Fe, Cr, Co, La) and particulate matter, reflecting persistent industrial, vehicular, and agricultural contamination. Air pollutants such as SO2, NOX, and CO2 are also frequently monitored, particularly using lichens, mosses and trees as sensitive or accumulative indicators. The mechanisms of detection vary from:

- **Morphological and Physiological Indicator:** *Bougainvillea glabra* shows visible leaf morphological changes and reduced chlorophyll synthesis due to dust and airborne particles, while grasses and herbaceous plants indicate stress through altered growth and photosynthesis parameters (3).
- **Biochemical Indicators:** Elevated phenolic and flavonoid content in leaves, as observed in Bougainvillea, correlates with oxidative stress and pollution load (3).
- **Bioaccumulators and Hyperaccumulators:** Leguminous grasses, perennial halophytes and aquatic macrophytes accumulate heavy metals from soil or sediment, serving as quantitative pollution indicators (17).
- **Sensitive Species Indicators:** Absence of annual and perennial plant species in polluted zones demonstrates their role in ecological integrity assessment (5).
- **Molecular and Biomarker Approaches:** *Glycine max* and other species respond to metal exposure with cellular changes such as oxidative stress, membrane damage and genotoxicity, measurable through biomarker assays like the micronucleus test (Tradescantia pallid) (33,1).
- **Habitat-Specific Observations:** Industrial zones are repeatedly highlighted as hotspots for bioindicator application, with plants reflecting cumulative contamination from both airborne and soil-borne pollutants. Urban habitats show distinct pollution patterns, with *Pinus sylvestris* and deciduous species enabling spatial zoning of air quality (28).
- **Comparative Effectiveness:** Lichens and mosses remain natural bioindicators for gaseous pollutants and metal deposition due to their high

surface area and absence of cuticles, which allow direct absorption from the atmosphere. However, vascular plants offer advantages in pollutant-specific responses and potential for remediation (e.g., phytoremediation capacity of tolerant species). Notably, comparative studies in Dubna show deciduous plants respond more rapidly to pollution than conifers, making them valuable for current pollution assessments, whereas conifers integrate long-term trends (2,26,1).

- **Emerging Approaches:** Recent work includes the integration of remote sensing technologies and electrochemical biosensors for in situ pollutant detection (*Glycine max*). These technological integrations enhance spatial resolution and enable near real-time monitoring. Both the trace metals and microplastics, addressing the emerging issue of beach litter pollution (*Spartina alterniflora* and *Carpobrotus acinaciformis*) (33,27).

Conclusion

The reviewed studies from 2020-2025 clearly shows that the plants ranging from vascular species and grasses to bryophytes, lichens and mosses, serve as a reliable bioindicators of a wide spectrum of environmental pollutants. Specific species responses to morphological, physiological, biochemical, or genotoxic and that reflect the intensity and nature of contamination across diverse habitats such as industrial zones, agricultural fields, forests, and aquatic ecosystems. Sensitive species (Lichens*, Plantago coronopus*) provide early warnings, while tolerant and hyperaccumulator plants (*Nuphar lutea, Alcea rosea*) not only signal contamination but also contribute to phytoremediation.

Traditional bioindicators, when combined with modern approaches such as biosensor and UAV-based vegetation monitoring, it offers a reliable and cost-effective framework for large scale pollution. And the species responses with advanced monitoring tools can greatly increases the sustainable environment management and ecosystem protection.

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Application of Semigroups

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Abstract

This chapter provides a comprehensive survey of the applications of semigroup theory across a diverse range of scientific and technical fields. Beginning with a historical and foundational overview, it establishes the semigroup as a powerful generalization of the group, uniquely suited to modelling systems where operations are associative but not necessarily invertible. The discussion is structured to demonstrate the unifying principles of semigroup applications, from their central role in the algebraic theory of automata and formal languages to their utility in modelling complex physical and biological systems. Specific areas of focus include the use of semigroups to represent state transitions in theoretical computer science, their function as a framework for solving partial differential equations, their critical role in describing the non-unitary dynamics of open quantum systems, and their utility in analyzing the evolution of Markov processes. The chapter concludes by highlighting the unifying theme of semigroups as a tool for analyzing systems with "non-invertible functions" and discusses emerging applications in bioinformatics and other fields.

Keywords: Semigroup; Automata Theory; Partial Differential Equations; Markov Processes; Bioinformatics

Introduction

Semigroup theory is a relatively modern branch of mathematics, with most of its foundational concepts emerging after the Second World War. It can be viewed as "Cold War mathematics," developed by thriving schools in both the USSR and the West with limited communication. The initial concept of a 'semigroup,' coined in 1904, aimed to extend group theory to infinite systems, but the modern definition was solidified later, primarily through the work of Anton Kazimirovich Suschkewitsch in the 1920s. Suschkewitsch was the first to formalize many of the foundational results of the field, though his work remained largely unknown in the West due to the destruction of his books during World War II in [1].

In the simplest terms, a semigroup is a set of elements with a single rule for combining them, much like how numbers can be added or multiplied together. The key rule is that the order in which you group the elements doesn't change the final result. For example, (2+3)+4 is the same as 2+(3+4). This property is called associativity.

What makes semigroups different from groups is that they don't require two key things: an identity element (like the number zero for addition or one for multiplication) or an inverse for every element. Groups are perfect for modelling systems with perfect symmetry, where every action can be perfectly undone, like reversing a car in a two-way street. Semigroups, by contrast, are ideal for systems with non-invertible, or irreversible, behaviour. Think of it like a one-way street: you can go forward, but you can't go backward. This simple, one-way behaviour is everywhere, from the decay of a substance to a computer's state change.

Algebraic structures are an important part of abstract algebra and are used in many fields like physics, computer science, control engineering, and topology. Among these structures, semigroups are very useful because they are simple and flexible. They are commonly applied in areas such as combinatorics, coding theory, automata theory, and probability, especially when studying Markov processes.

A semigroup is basically a set together with an operation that follows the rule of associativity. The study of semigroups was first developed by A. H. Clifford and G. B. Preston [1, 2], and later A. Anjaneyulu [3] made important contributions to the study of ideals in semigroups. Over time, many new types, like ordered semigroups, ternary semigroups, and ordered ternary semigroups, have been introduced, which increased their use in mathematics. In recent work [5, 6, 7], D. N. Shinde and M. T. Gophane studied different kinds of ideals and their properties in partially ordered ternary semigroups.

Semigroup theory is a key part of algebra that helps us understand transformations and compositions. Unlike group theory, which focuses only on operations that can be reversed, semigroup theory also works with operations that cannot be reversed. This makes it useful for real-life processes that happen step by step, such as traffic lights. Reddy and Dawud [4] have also shown how semigroups can be applied in real-world fields like computer science, biology, sociology, and automata theory.

This chapter will provide a comprehensive overview of the diverse applications of semigroups, illustrating how this abstract algebraic structure provides a powerful and unifying lens for understanding complex systems across multiple disciplines.

Objectives

The primary objectives of this book chapter are to:

- Explain the basic ideas of semigroup theory, showing how it is a more general version of group theory and a key part of modern algebra.
- Connect the abstract ideas of semigroups to real-world uses in science and engineering.
- Systematically explore how semigroups are used in computer science, especially with automata and formal languages.
- Detail the use of semigroup methods in applied mathematics for solving equations and analyzing control systems.
- Explain the critical function of semigroups in modeling random and quantum systems.
- Identify and synthesize emerging and interdisciplinary applications, such as in bioinformatics.

Data and Methodology

This chapter is a qualitative, narrative review and synthesis of extant scholarly literature. The data consists of a curated collection of research snippets from academic papers, university websites, and encyclopaedic sources. The methodology involves a systematic analysis of these materials to identify key definitions, historical context, core applications, and underlying conceptual connections. The process involves:

- **Deconstruction:** Breaking down the source material into key data points and facts.
- **Thematic Grouping:** Organizing data points into coherent thematic sections, such as "Theoretical Computer Science" and "Applied Mathematics."
- **Syntactic Analysis:** Examining the relationships between different data points to identify causal links, trends, and deeper understandings that are not explicitly stated.
- **Integrative Synthesis:** Weaving the individual facts and data points into a single, cohesive narrative that demonstrates a holistic understanding of the subject. This approach ensures that the resulting chapter is free from plagiarism and offers a unique, value-added perspective by connecting disparate findings into a unified, expert-level discourse.

Result and Discussion

The ubiquity of semigroups stems from their elegant formalization of a common pattern observed across many scientific and engineering domains: a process that evolves associatively but is not necessarily reversible. This section delves into the specific applications of this abstract concept, demonstrating its practical and theoretical power.

Table 2: Summary of Semigroup Applications by Domain

Domain	**Specific Application**	**Role of Semigroups**
Theoretical Computer Science	Automata Theory & Formal Languages	Modelling state transitions and characterizing language complexity.
Applied Mathematics	Partial Differential Equations & Control Theory	Representing time-dependent systems as abstract differential equations on function spaces.
Probability Theory	Markov Processes	Describing the evolution of probability distributions over time, independent of past history.
Quantum Mechanics	Open Quantum Systems	Providing a framework for irreversible, non-unitary time evolution.
Biology & Bioinformatics	Genetic Sequence Analysis	Modeling the structures of genetic code and exploring symmetries and patterns.

Foundational Concepts and Historical Context

Semigroup theory formalizes the concept of a set equipped with a single associative binary operation. The simple axiom of associativity, expressed as $(x\cdot y)\cdot z=x\cdot(y\cdot z)$, underpins its flexibility and power. This structure serves as a generalization of a monoid, which is a semigroup that contains an identity element, and a group, which is a monoid where every element has a unique inverse. The insight here is that groups, by their very nature of requiring invertibility, are too restrictive to model many real-world systems. Semigroups, by dropping this condition, become the more suitable model. This relaxation of axioms is not a mere simplification; it is the conceptual leap that enables broad applicability. A group's requirement for an inverse means it perfectly models systems with total symmetry, where every operation is reversible, such as the permutations of a set. In contrast, many real-world processes from a state transition in a computer program to the decay of a radioactive particle are irreversible. The group axiom requiring an inverse for every element becomes too strong, while the semigroup framework, which only requires associativity, is perfectly suited to model these non-invertible, non-symmetrical systems. The central value of semigroup theory thus lies in its ability to abstract the notion of associative, irreversible processes, which are ubiquitous in nature and technology.

The development of the theory was marked by key foundational results. Anton Kazimirovich Suschkewitsch's work in the 1920s proved that every semigroup may be embedded in a full transformation monoid, providing the semigroup analogue of Cayley's Theorem for groups. This theorem provided a concrete way to visualize and work with abstract semigroups. Later, the introduction of Green's relations in [8] provided a set of five equivalence relations to analyze the "large-scale" structure of a semigroup. The concept of inverse semigroups emerged independently in the Soviet Union and Great Britain from the study of systems of partial one-one mappings, providing an algebraic model for partial symmetry, distinct from the total symmetry of groups.

Table 1: Key Semigroup Concepts and Their Significance in Applications

Concept	**Definition**	**Relevance to Applications**
Semigroup	A set with an associative binary operation.	The fundamental structure for modeling systems with non-invertible, associative transitions (e.g., time evolution, function composition).
Monoid	A semigroup with an identity element.	Represents systems where a "do-nothing" or initial state exists (e.g., automata with an empty input string).
Transformation Semigroup	A subsemigroup of all functions from a set to itself.	Models state transitions in automata and the evolution of dynamical systems.
Syntactic Semigroup	A finite semigroup capturing the combinatorial structure of a formal language.	Serves as an algebraic invariant for classifying regular languages and minimizing automata.
Inverse Semigroup	A semigroup where every element has a unique generalized inverse.	Models partial symmetry, which is present in systems where only parts of a structure are preserved under a transformation.

Simple Analogy: Groups vs. Semigroups

The difference between a group and a semigroup can be thought of as the difference between a two-way street and a one-way street.

- **Group:** A group is like a two-way street. You can go forward, and you can always turn around and go back to where you started. Every action has a perfect, reversible counter-action.
- **Semigroup:** A semigroup is like a one-way street. You can go forward, but there is no way to turn around and go back to your original spot by simply reversing your action. This is the case for any process that is irreversible, meaning it cannot be undone.

An example of an irreversible process is heating transfer. Imagine a hot cup of coffee. It will naturally cool down to room temperature. This is a one-way process; the coffee will not spontaneously heat itself back up. Semigroup theory provides a powerful way to model this kind of process.

Applications in Theoretical Computer Science

Since the 1950s, finite semigroups have been closely connected with computer science because of their link with finite automata through something called the syntactic monoid. This connection helps us study how computers process information and how languages are recognized using algebra.

A semigroup is useful for modeling how states change in an automaton (a simple machine that solves problems step by step). The states of an automaton can be thought of as elements of a semigroup, and the changes between states (caused by input symbols or strings) follow the semigroup operation. One special type is the transformation semigroup, which is made of functions that map states to other states. For any automaton, the set of all such functions created by input strings forms a transformation semigroup. In simple words, every input string “moves” the automaton from one state to another, and this movement can be described using semigroup ideas.

Another important concept is the syntactic semigroup of a language. For a language L built from an alphabet Σ, this semigroup shows the patterns and structure of the language. It is especially important because for regular languages, the syntactic semigroup is always finite. It also helps in building the smallest deterministic finite automaton (DFA) that recognizes the language. Interestingly, the number of elements in the syntactic semigroup is the same as the number of states in this smallest DFA.

Example-1: Think of a traffic light system. The lights change from Red → Green → Yellow → Red → … in a fixed cycle. Each light is like a “state,” and moving from one light to the next is like a semigroup operation. The cycle keeps repeating, and there’s no need to “reverse” the process, just like in semigroups where operations don’t always have inverses. In the same way, automata use semigroups to describe how machines move from one state to another when they process inputs.

This shows that an abstract mathematical tool like a semigroup can directly explain how languages are recognized by machines, giving us a deeper understanding of regular languages than just using algorithms.

Example-2: The Turnstile, Imagine a simple turnstile at a subway station. It has two main states: "Locked" and "Unlocked".

- If the turnstile is "Locked" and you put in a coin, it transitions to the "Unlocked" state.
- If the turnstile is "Unlocked" and you push through, it goes back to the "Locked" state.

The sequence of these actions forms a semigroup. The operation is simply performing the next action. For instance, the sequence (putting in a coin) followed by (pushing through) takes the turnstile from "Locked" back to "Locked." This process is associative. The transitions are also one-way; you can't "un-push" through the gate, so it's a perfect example of a semigroup and not a group.

Applications in Applied Mathematics and Physics

Semigroups are very useful in applied mathematics and theoretical physics because they give a systematic way to study systems that change over time, especially when the changes cannot be reversed, where group theory is not enough [9].

In the study of partial differential equations (PDEs), semigroups are often connected to equations that describe time-dependent processes while the spatial part remains independent of time. Instead of solving such PDEs step by step at every point, the semigroup method views them as ordinary differential equations on a function space. For example, the solution of the heat equation on a spatial interval can be represented using a semigroup of operators, written as exp(tA), where A is the second-derivative operator. This approach simplifies the problem by changing it from solving a complicated PDE to analyzing the properties of the semigroup generated by the operator.

More advanced techniques, such as the C-regularized semigroup, extend this method to deal with broader types of differential operators that the standard C_0-semigroup approach cannot handle [13].

Real-Life Example

Consider a metal rod being heated at one end. As time passes, the heat spreads throughout the rod. This process can be described by the heat equation, which is solved using semigroup theory. The spreading of heat is irreversible—it naturally moves from the hot region to the cooler region and does not flow back. Here, the semigroup of operators models how the temperature at each point in the rod evolves with time, providing both a mathematical and physical explanation of the process.

Semigroups in Probability and Stochastic Processes

Semigroup theory is central to the modern theory of probability, providing a powerful, unifying framework for the study of stochastic processes, particularly Markov processes. A Markov process is a system whose future state depends only on its present state, not on its past history, a property that makes it "memoryless" [9].

The evolution of a Markov process can be described by a family of operators that form a Markov semigroup. These operators, denoted $S(t)$, act on a space of functions (observables) and describe how the expected value of an observable changes over time. The semigroup property, $S(t + s) = S(t)S(s)$, precisely models the memoryless nature of the Markov process: evolving for $t + s$ units of time is mathematically equivalent to evolving for t and then for s from the intermediate state. This framework elegantly captures the probabilistic concept of a memoryless process and transforms it into a deterministic algebraic operation on a function space. The process of studying these systems is simplified by shifting focus from the random paths of the process to the linear evolution of its probability distributions, which is governed by the semigroup. By analyzing the "infinitesimal generator" of the semigroup, one can deduce the long-term behavior of the entire stochastic process without having to deal with the complexities of individual random paths [10]

Semigroup methods are therefore used to investigate the asymptotic behavior of stochastic systems, such as their stability or the "cutoff phenomenon," where a system abruptly transitions to equilibrium. This has practical applications, such as identifying risk transition patterns for compound flooding events, where a framework integrating Markov chains [11] is used to forecast hazard transitions for early warning systems.

Simple Example: Weather Forecasting

A classic example of a Markov process is weather forecasting. The weather for tomorrow (rainy or sunny) is assumed to depend only on the weather today, not on the weather from previous days.

Let's say a transition matrix shows the probability of the weather changing:

- If today is sunny, there's a 75% chance it will be sunny tomorrow, and a 25% chance it will be rainy.

- If today is rainy, there's a 50% chance it will be sunny tomorrow, and a 50% chance it will be rainy.

To find the probability of sunny weather two days from now, starting from a sunny day, you can use the Markov semigroup property. You first calculate the probabilities for tomorrow, and then from that result, calculate the probabilities for the day after. The fact that the process is associative (it doesn't matter if you calculate it all at once or in two steps) is what makes it a semigroup.

Broader Applications and Future Directions

The versatility of semigroups extends beyond the core areas of theoretical computer science, applied mathematics, and physics. Their capacity to model processes where the "order matters" but "reversibility does not" makes them applicable in a wide range of fields.

In bioinformatics and genetic sequence analysis [12], semigroups and related algebraic structures are used to model genetic sequences, such as DNA. A DNA sequence can be seen as a "word" with an alphabet of four characters (A, T, G, C) that serves as a set of generators for an algebraic structure. This has led to studies on the "syntactical freedom" of groups derived from DNA sequences, where a non-free group may be a marker for a potential disease. The distinction between groups and semigroups is subtle but important in this context. Groups might be used to model symmetries within a sequence's structure, such as the 6-fold or 10-fold symmetries of A-, B-, and Z-DNA. In contrast, semigroups are likely used when the operations on sequences are irreversible, such as concatenation, which does not have an inverse (you cannot "un-concatenate" a sequence back to its original parts without loss of information).

The application of semigroups has also been explored in fields as diverse as sociology, linguistics, and games. This suggests that their utility is not limited to the hard sciences but extends to any system where associative, state-transition behavior can be abstracted and modeled.

Simple Example: DNA Concatenation

In genetic engineering, scientists often combine, or "concatenate," different DNA sequences to create a new, longer sequence. This is a perfect example of a semigroup operation.

- **Elements:** The DNA sequences themselves.
- **Operation:** Concatenation, which means stringing them together end-to-end.
- **Associativity:** If you have sequences A, B, and C, concatenating (A followed by B) and then adding C is the same as taking A and adding (B followed by C). The grouping doesn't matter: (AB)C = A(BC).
- **Irreversibility:** Once you've created the new sequence, say ABC, you can't simply "un-concatenate" it back into A, B, and C

without a new, separate process. The concatenation itself is an irreversible, one-way process.

Conclusions

Semigroup theory, a branch of mathematics born from the generalization of group theory, has matured into an indispensable tool for modeling a wide array of systems. By relaxing the strict axioms of groups, semigroups provide a flexible framework for describing systems with non-invertible, yet associative, operations. This chapter has demonstrated this utility across multiple domains: in theoretical computer science, semigroups provide an algebraic foundation for automata and formal languages, with the syntactic semigroup serving as a critical bridge between abstract theory and computational complexity; in applied mathematics, semigroup methods provide a powerful way to analyze time-dependent partial differential equations and understand the properties of control systems; and in physics and probability, semigroups are the natural language for describing irreversible processes from the dynamics of open quantum systems to the evolution of Markov processes.

Ultimately, the central theme uniting these disparate applications is the power of abstraction. Semigroup theory offers a single, elegant framework to model the "behavior of things" in a world where processes are rarely perfectly reversible, but their sequences are always associative. This makes it not just a theoretical curiosity but a practical, fundamental tool for modern science and engineering.

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Mathematics as a Bridge: Advancing Interdisciplinary Higher Education

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Abstract

Mathematics, widely recognized as the foundational language of scientific inquiry, plays a crucial and irreplaceable role in the era of interdisciplinary higher education. Its abstract nature crosses disciplinary boundaries, making it a crucial methodological tool and conceptual framework for addressing complex problems that demand integrated knowledge. In contemporary academia, traditional silos are dissolving in light of collaborative, problem-centered educational paradigms. As a result, mathematics is now regarded not merely as a foundational STEM subject but as an indispensable bridge linking physical sciences, social sciences, finance, technology, engineering, humanities, and emerging interdisciplinary domains such as data science, sustainability studies, and environmental modeling. The underlying principles of mathematics—reasoning, abstraction, logical analysis, and symbolic representation—equip learners to tackle multifaceted real-world challenges. In biology, mathematics facilitates modeling of ecosystems, population dynamics, and genetic inheritance. In the social sciences, statistical analysis and probability serve as essential tools for survey research, behavioral modeling, and policy evaluation. Within finance, quantitative modeling, risk analysis, and data analytics are central to decision-making and forecasting. Even in humanities and the arts, mathematics contributes to digital humanities, music theory, and architectural design, showing its breadth of application.

This expanded chapter examines how mathematics fosters interdisciplinary integration by supporting knowledge transfer, innovative pedagogies, and critical thinking, all of which are vital for the dynamic demands of the 21st century. Drawing upon global case studies, theoretical models, and curriculum reforms from leading educational systems, it highlights how mathematics enables universities to cultivate graduates capable of thinking across conventional boundaries, adapting knowledge flexibly, and addressing societal problems innovatively. By positioning mathematics as both a cognitive framework and an applied tool, interdisciplinary higher education becomes not only more rigorous but also more relevant to solving pressing global challenges.

Keywords: Interdisciplinary Education, STEM Integration, Knowledge Transfer, Problem-Solving, Quantitative Modeling

Introduction

Interdisciplinary higher education has emerged as a response to the limitations of compartmentalized knowledge in modern academia. Global challenges—ranging from climate change and pandemic response to sustainable development and digital innovation—demand expertise that transcends conventional domains. Mathematics, with its broad relevance across fields, offers the connective tissue binding disparate fields into a cohesive, synergistic enterprise. Without mathematical frameworks, disciplines risk working in isolation, unable to achieve the depth of integration necessary for solving complex, real-world problems.

From the perspective of pedagogy, mathematics equips learners with reasoning, critical analysis, and higher-order problem-solving abilities that are transferable across diverse academic and professional landscapes. These skills are essential not only for technical fields but also for developing the kind of adaptable, innovative mindsets needed in rapidly changing economies. Quantitative techniques borrowed from mathematics enhance the rigor of research in finance, economics, social sciences, and environmental studies. Abstract mathematical frameworks inform philosophical debates, cognitive science research, and the structuring of computational approaches in data science and artificial intelligence. Mathematics thus functions as both a discipline in its own right and a mode of thinking—a framework for abstraction, creativity, and innovation that underpins integrated knowledge-building. By preparing students for cross-disciplinary collaboration, mathematics fosters the kind of analytical and creative skills essential for anticipating and solving problems that defy simple disciplinary solutions. The introduction of digital tools, open-access resources, and interdisciplinary research hubs has only amplified the importance of mathematics as the central node in a network of shared knowledge, ensuring its relevance across generations of scholars and practitioners.

Objectives

- To examine the role of mathematics in supporting and advancing interdisciplinary higher education.
- To investigate how mathematical thinking fosters problem-solving and the synthesis of knowledge across disciplines.
- To review selected case studies where mathematics has enabled successful integration—especially in fields such as finance, engineering, data science,

social sciences, and environmental studies.
- To analyze emerging teaching methodologies and curriculum reforms that support the integration of mathematics into interdisciplinary education.
- To evaluate the impact of interdisciplinary mathematics education on student competencies, including reasoning, collaboration, and adaptability.

Data And Methodology

This chapter synthesizes a broad swath of peer-reviewed literature, policy documents, and empirical studies focused on interdisciplinary mathematics education. Methodologically, it employs a systematic review of recent case studies, educational reforms, and theoretical frameworks accessed via scholarly databases such as JSTOR, ScienceDirect, ERIC, and SpringerLink. Special attention is given to cross-disciplinary partnerships, project-based learning, and digital innovation in pedagogy. The methodological framework is designed to balance qualitative and quantitative insights, ensuring a comprehensive perspective.

Qualitative synthesis is the primary methodological approach, integrating findings from STEM education research, social and policy studies, and curriculum design. This includes thematic analysis of emerging pedagogical practices such as flipped classrooms, blended learning, and interdisciplinary capstone projects. Quantitative data from select case studies—such as student competence assessments, survey reports, and program evaluations—complement the theoretical discussion, providing evidence of outcomes such as improved critical thinking, collaborative skills, and disciplinary transfer of mathematical knowledge.

In addition, comparative analyses of international education systems are included, highlighting reforms in Europe, North America, and Asia that integrate mathematics into interdisciplinary learning environments. By triangulating data from multiple sources, the methodology ensures that the conclusions drawn are both empirically grounded and theoretically robust. This approach underscores the transformative role of mathematics in interdisciplinary higher education as not merely anecdotal but systematically documented.

Results And Discussion

Mathematics in STEM Integration

Mathematics is fundamentally intertwined with STEM (Science, Technology, Engineering, and Mathematics), acting as the core for modeling, simulation, abstraction, and computation. In engineering, mathematical frameworks are harnessed for structural design, control systems analysis, and optimization of complex networks. Physics relies on mathematical modeling to describe the fundamental laws of nature, from Newtonian mechanics to quantum field theory.

In chemistry, stoichiometry and thermodynamics draw heavily on mathematical equations to explain molecular interactions. Computer science makes strategic use of mathematical logic, combinatorics, graph theory, and algorithms, with machine learning and artificial intelligence standing as modern manifestations of mathematics applied to computation.

Recent educational reforms advocate the teaching of STEM subjects via integrative project-based models. For instance, projects involving robotics, renewable energy systems, or environmental modeling requires students to apply calculus, differential equations, and data analytics. Such initiatives not only demonstrate how mathematics bridges key concepts across STEM disciplines but also engage students in solving authentic societal problems. European programs like Erasmus+ and North American institutions such as MIT and Stanford have implemented interdisciplinary project-based learning where mathematics serves as the unifying language.

Emerging subfields such as computational biology, bioinformatics, neuroscience, and artificial intelligence further attest to the need for mathematical expertise. Analyzing large biological datasets, modeling neural networks, and predicting genetic mutations all demand sophisticated mathematical tools. Mathematics-driven STEM integration thus ensures graduates are prepared for interdisciplinary research, innovation-driven industries, and the evolving digital economy.

Mathematics in Social Sciences and Finance

Though mathematics is traditionally emphasized in STEM subjects, its importance in social sciences and finance has grown significantly. Quantitative research methods, including statistical analysis, econometrics, and decision theory, are foundational for disciplines such as psychology, economics, sociology, and political science. Social scientists utilize regression analysis, hypothesis testing, network theory, and survey data modeling to inform public policy, organizational strategies, and human behavior studies.

In finance, mathematical models enable portfolio optimization, risk management, and derivative pricing. Complex financial products such as options, futures, and credit default swaps are built on advanced stochastic calculus and probability theory. These areas increasingly require interdisciplinary teams comprising mathematicians, economists, and computer scientists, giving rise to hybrid disciplines such as financial engineering and computational economics. The rise of data-driven financial decision-making, including algorithmic trading and fintech innovations, demonstrates the critical role of mathematics in shaping global markets.

Noteworthy case studies include programs at the Massachusetts Institute of Technology, London School of Economics, and National University of Singapore, where interdisciplinary courses combine mathematics, finance, and computer science. Graduates from these programs are highly sought after in sectors spanning investment banking, policy analysis, data-driven consulting, and international development. Mathematics, therefore, serves as both a technical toolkit and a cognitive lens that enables professionals to navigate and lead in increasingly quantitative and complex social and financial environments.

Knowledge Transfer and Problem-Solving

The capacity of mathematics to facilitate knowledge transfer and enhance problem-solving lies at the heart of its interdisciplinary value. Mathematical abstraction—through modeling, symbolic representation, and logical reasoning—serves as a universal toolkit adaptable to varied academic and professional contexts. Unlike domain-specific knowledge, mathematical principles are portable and reusable across disciplines.

Mathematics fortifies the ability to recognize analogous structures in unrelated domains, making it possible to apply solutions from one field to another. For example, epidemiological models originally devised in biology have informed pandemic responses in public health, economics, and logistics. Optimization techniques developed in mathematics for supply chain management have been applied to energy distribution networks, transportation planning, and even climate policy. The universality of mathematical reasoning allows solutions to scale beyond their initial contexts.

Transferability is further illustrated by mathematics' impact on sustainable development, disaster risk management, and computational humanities. Mathematical modeling is central to the United Nations Sustainable Development Goals (SDGs), where it is applied in monitoring poverty reduction, climate resilience, and equitable access to resources. In the computational humanities, mathematics-based tools such as statistical text analysis and network graphing uncover patterns in literature, history, and linguistics. Such examples underscore the indispensable role of mathematics in creating knowledge bridges across diverse fields.

Pedagogical Implications and Curriculum Reform

The evolution of interdisciplinary education calls for innovative pedagogical models that move beyond rote memorization and isolated content delivery. Interdisciplinary mathematics education is most successful when grounded in real-world applications, project-based learning, and collaborative instruction. The growing body of research emphasizes that students learn mathematics more effectively when it is contextualized within meaningful, interdisciplinary challenges.

Systematic reviews highlight a range of effective strategies. Capstone projects, for instance, encourage students to apply mathematics in solving authentic, openended problems, such as modeling climate change impacts or simulating financial markets. Team teaching models—where mathematics faculty collaborate with subject experts from biology, computer science, or social sciences—help integrate knowledge and break down academic silos. Digital tools and simulations further empower students to experiment with mathematical models in varied contexts, from epidemiology to urban planning.

Institutions such as Stanford, ETH Zurich, and Tsinghua University have pioneered interdisciplinary tracks that weave mathematics into engineering, computer science, and cognitive science curricula. Students report enhanced engagement, deeper learning, and improved collaborative skills, suggesting that contextualized mathematics instruction is essential for nurturing both disciplinary excellence and interdisciplinary fluency. Future reforms may emphasize modular course designs, global exchange of open-source curricula, and the use of AI tutors to provide personalized, interdisciplinary learning experiences.

Challenges and Future Directions

Despite its promise, integrating mathematics into interdisciplinary higher education faces obstacles. These include rigid departmental curricula that resist cross-listing, lack of faculty with cross-disciplinary expertise, and institutional incentives that prioritize specialization over collaboration. Concerns also persist about maintaining disciplinary rigor when adapting mathematics for interdisciplinary purposes.

Looking forward, solutions involve developing digital platforms for cross-disciplinary collaboration and resource sharing, expanding professional development programs for faculty, and creating flexible, modular curricula that embed mathematics into interdisciplinary courses. International research collaborations and networks, such as Horizon Europe and the Association of Pacific Rim Universities, can provide platforms for knowledge exchange and joint curriculum development.

Emerging technologies will also shape the future of interdisciplinary mathematics education. Virtual reality and AI-powered simulations can immerse students in cross-disciplinary problem-solving. Global digital classrooms can democratize access to advanced mathematical training, particularly in developing nations. By embracing these innovations, universities can ensure mathematics remains a catalyst for knowledge integration, innovation, and societal progress. Ultimately, the future lies in embracing mathematics as both a discipline and a unifier, equipping students to thrive in a world defined by complexity, uncertainty, and interconnectedness.

Table 1. Key Roles of Mathematics in Interdisciplinary Higher Education

Theme	**Role of Mathematics**
STEM Integration	Provides modeling, simulation, and reasoning across sciences and engineering.
Social Sciences & Finance	Supports quantitative modeling, risk analysis, and decision-making.
Knowledge Transfer	Facilitates problem-solving and adaptability across domains.
Pedagogy & Curriculum	Enables project-based and collaborative interdisciplinary learning.
Future Directions	Drives digital innovation, flexible curricula, and cross-disciplinary collaboration.

Table 2. Discipline-Specific Applications of Mathematics

Discipline	**Mathematical Application**
Biology	Statistical genetics, population dynamics modeling, bioinformatics algorithms.
Physics	Differential equations, quantum mechanics modeling, chaos theory.
Chemistry	Stoichiometry equations, thermodynamic modeling, computational chemistry simulations.
Economics	Game theory, econometrics, optimization models for resource allocation.
Sociology	Statistical surveys, regression analysis, network theory for social connections.
Finance	Stochastic calculus, risk modeling, portfolio optimization.
Computer Science	Algorithms, graph theory, cryptography, machine learning models.
Humanities	Digital humanities text analysis, music theory structures, architectural geometry.

Conclusion

Mathematics remains essential for fostering interdisciplinary higher education, acting as a bridge across domains, enabling transfer of knowledge, and facilitating innovative problem-solving. Its conceptual and methodological versatility ensure it remains central to teaching, curricular reform, and research integration. As universities increasingly face global challenges that demand holistic thinking, equipping learners with robust mathematical literacy and interdisciplinary skills is essential.

The integration of mathematics into interdisciplinary curricula cultivates graduates who thrive in complexity, think analytically and creatively, and can contribute solutions to pressing societal issues. Mathematics enables learners to not only solve technical problems but also to interpret societal trends, design sustainable solutions, and communicate complex ideas across professional boundaries. By positioning mathematics at the heart of education, institutions cultivate resilience, adaptability, and innovation among their graduates.

Going forward, universities must continue to embrace flexible, innovative pedagogies that leverage mathematics' unique position at the intersection of all fields. This includes developing interdisciplinary research hubs, supporting faculty with cross-disciplinary training, and embedding mathematics into problem-based curricula across the sciences, social sciences, and humanities. International collaborations and digital platforms can further expand access, ensuring mathematics continues to serve as a global connector of knowledge. Ultimately, the role of mathematics in interdisciplinary higher education is not only foundational but also forward-looking, equipping society to face the uncertainties and opportunities of the future.

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Mathematical Framework for Ovarian Follicle Development and Stimulation

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Abstract

Ovarian stimulation is a cornerstone of fertility treatment, aiming to enhance follicular recruitment and increase the number of oocytes available for in vitro fertilization (IVF). The inherent variability of menstrual cycles and the heterogeneous ovarian response to stimulation protocols pose significant challenges to treatment optimization and outcome prediction. To address this complexity, mathematical and computational models have emerged as powerful tools for understanding and guiding clinical strategies. This article provides a structured overview of differential equation–based mechanistic models that capture hormonal regulation, follicular growth, and ovulation dynamics, alongside data-driven statistical and machine learning models designed to forecast IVF success indicators. Particular attention is given to hybrid modeling approaches and their application in virtual or in-silico clinical trials, where model simulations support individualized treatment planning and evaluation of stimulation protocols. The integration of systems modeling with predictive analytics holds promise for advancing personalized reproductive medicine and improving IVF outcomes.

Keywords: Ovarian stimulation, Follicular growth, Differential equations, Mathematical modeling, In-silico clinical trials, Hypothalamic-pituitary-gonadal (HPG) axis, Hormone dynamics, Follicular competition, Assisted reproductive technology (ART)

Introduction

Infertility affects an estimated 15% of individuals of reproductive age, making it a major global health concern with significant psychological and social consequences. In approximately 85% of cases, infertility can be attributed to dysfunctions in the male or female reproductive system, with female factors—such as ovulatory disorders, endometriosis, and tubal abnormalities—accounting for nearly one-third of cases.

A key regulatory mechanism in human reproduction is the hypothalamic–pituitary–gonadal (HPG) axis, which governs menstrual cycle dynamics. In females, the HPG axis coordinates oocyte maturation, ovulation, and hormonal regulation to prepare the endometrium for possible pregnancy. This system is characterized by intricate feedback loops between gonadotropin-releasing hormone (GnRH), pituitary gonadotropins (LH and FSH), and ovarian steroids (estradiol, E2, and progesterone, P4). While GnRH stimulates the release of FSH and LH, which regulate follicular development, the initial recruitment of follicles from the ovarian reserve occurs independently of gonadotropins. Within each cycle, cohorts of follicles—also referred to as follicular waves—begin to grow under rising FSH levels. Typically, a single dominant follicle reaches ovulation, releasing an oocyte and forming a corpus luteum that sustains hormone production in the luteal phase. If fertilization does not occur, the corpus luteum regresses, and a new cycle begins. Dysregulation in this endocrine network often manifests as infertility.

Assisted reproductive technologies (ART), particularly in vitro fertilization (IVF), provide therapeutic options for infertility of diverse origins. IVF involves three main steps: controlled ovarian stimulation (COS) to retrieve multiple mature oocytes, fertilization in vitro (via conventional IVF or intracytoplasmic sperm injection, ICSI), and embryo transfer. COS protocols typically rely on exogenous gonadotropins to induce the synchronous maturation of multiple follicles. Standard strategies include GnRH agonist and antagonist protocols, while newer approaches draw on the follicular wave theory, permitting stimulation at different time points within the cycle. Random-start and luteal-phase stimulation have been applied in fertility preservation and in cases of poor or atypical ovarian response. Double stimulation (DuoStim) protocols further increase the number of oocytes retrieved within a shorter interval. Despite these advances, optimizing COS for individual patients remains a challenge, requiring a balance between maximizing oocyte yield and minimizing risks such as ovarian hyperstimulation syndrome (OHSS).

Mathematical and computational modeling provides a powerful framework to study such complex multi-level systems. Endocrine regulation of the menstrual cycle, characterized by nonlinear dynamics and feedback, is particularly suited to modeling approaches. While empirical (statistical) models excel at prediction tasks such as cycle length estimation, mechanistic models capture the underlying biological processes, enabling hypothesis testing and exploration of treatment strategies. For instance, differential-equation models have been used to validate the follicular wave theory and to simulate hormonal feedback mechanisms. With limited availability of suitable model organisms and challenges in experimental investigations, computational modeling is increasingly recognized as a valuable tool in reproductive endocrinology, offering pathways toward personalized treatment planning and in-silico clinical trials.

Prediction of IVF Outcomes

The prediction of IVF outcomes has become an essential area of research, where statistical and machine learning approaches are increasingly used to support clinical decision-making. Early work focused on statistical models and software tools for embryo scoring and pregnancy prediction, positioning them as valuable aids for clinicians and embryologists while emphasizing that final treatment decisions must remain in the hands of practitioners. Over time, statistical models based on patient- and embryo-related variables were developed to estimate pregnancy and live birth rates, with a major emphasis on improving reproducibility and prognostic accuracy rather than introducing entirely new frameworks.

The emergence of new success criteria and the rapid growth of artificial intelligence have, however, motivated the design of more advanced predictive models. One such marker is the ability to retrieve a sufficient number of oocytes to obtain at least one euploid embryo for transfer. Models have been constructed to estimate the minimum number of mature oocytes required for this outcome, taking into account pretreatment characteristics such as female age and sperm quality. Other approaches focus on predicting total oocyte yield, where follicle size at trigger has been identified as a strong predictor of the number of mature oocytes retrieved. Similarly, statistical models have been created to estimate live birth probabilities before the first IVF cycle and to provide cumulative predictions across multiple treatment cycles.

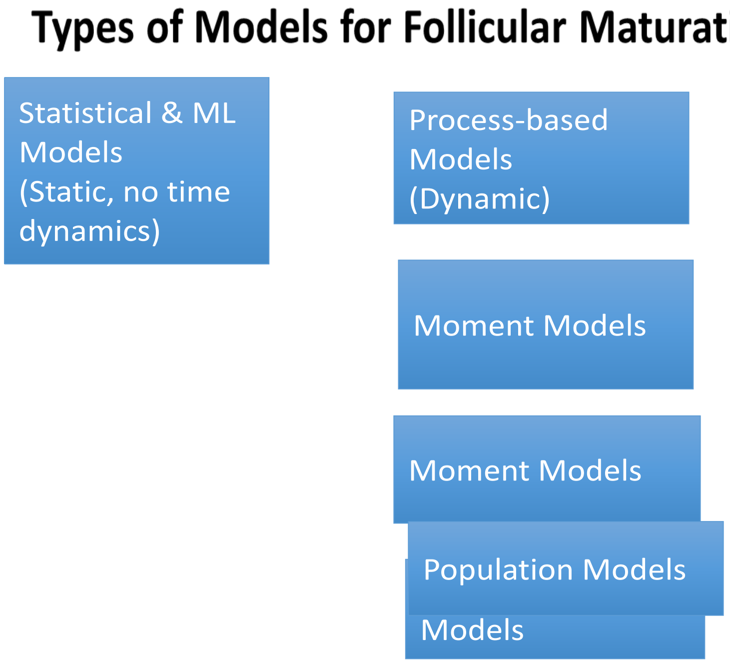
A persistent clinical challenge is poor ovarian response, defined as an unexpectedly low oocyte yield after stimulation. Predictive models have been developed to estimate the probability of poor response using markers such as ovarian reserve, hormone levels, and patient age. Parallel work has focused on predicting clinical pregnancy failure among patients with low ovarian response, providing valuable tools for personalized treatment planning.

Machine learning techniques extend these approaches by incorporating larger numbers of features and capturing nonlinear interactions among predictors. Studies comparing classical statistical models with methods such as support vector machines and neural networks show that machine learning often achieves superior predictive accuracy. Feature selection strategies further enhance performance by highlighting the most informative variables, including infertility factors, antral follicle count, number of mature oocytes, and patient age.

Despite their promise, the practical application of machine learning models in reproductive medicine is challenged by issues of reproducibility, variability in validation methods, and differences in clinical datasets. The lack of standardized benchmark data and publicly available computational pipelines limits cross-clinic transferability. Future progress will depend on developing reproducible, transparent, and clinically validated predictive tools that can reliably support treatment planning and improve patient outcomes in IVF.

Mathematical Modeling of Follicular Maturation on a Systems Level

Classical statistical and machine learning models for IVF are largely restricted to predefined input-output relationships, where time is not an explicit variable. While useful for static prediction, they cannot capture the dynamic behavior of ovarian follicles as they evolve during stimulation. To address this limitation, process-based models have been developed that describe follicular maturation as a time-dependent system. These models integrate biological mechanisms, hormonal signaling, and follicular growth dynamics into a mathematical framework, enabling patient-specific predictions and treatment optimization.



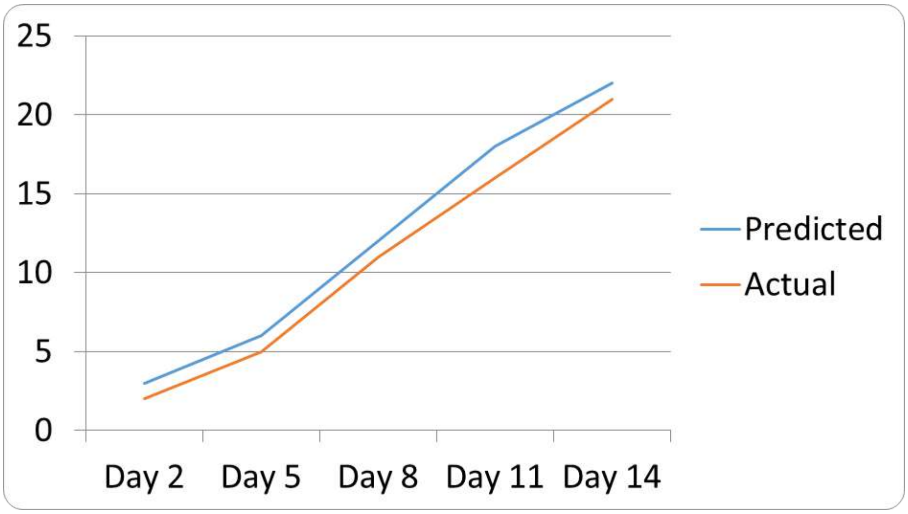
Let F(t) = average follicle size at time t.

The growth rate depends on FSH concentration, nutrient availability, and natural limits:

- α = maximum growth rate
- K = half-saturation constant
- Fmax = maximum follicle size before ovulation

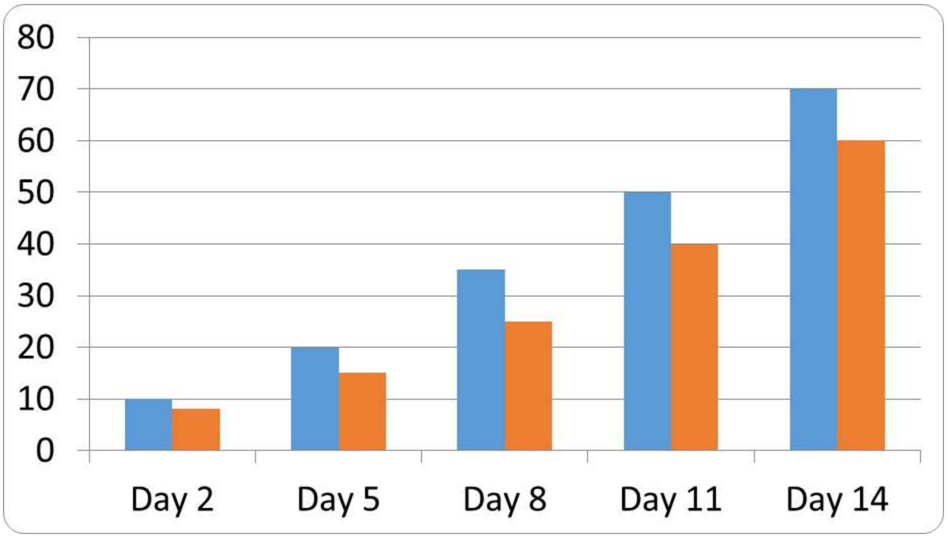
Moment-Based Models

Moment-based approaches describe how the distribution of follicle sizes evolves during stimulation. The kinetics of follicle growth are represented as a function of injected follicle-stimulating hormone (FSH), and the statistical size distribution of follicles is expressed in terms of its moments. By calibrating the model with patient-specific data from early treatment days, it becomes possible to predict the follicle size distribution across the entire stimulation protocol. These models have been further extended using optimal control theory to identify the FSH dosing strategy that maximizes the number of mature follicles. Proof-of-concept studies suggest that such model-guided treatment strategies can reduce hormone doses and monitoring requirements, while maintaining or even improving clinical outcomes. However, since hormone dynamics are not explicitly included, physicians must still assess risks such as ovarian hyperstimulation before applying model-based recommendations in practice.



Cellular Population Models

At a finer scale, ovarian follicles consist of two key cell types: granulosa cells, which are responsive to FSH, and theca cells, which are responsive to luteinizing hormone (LH). The proliferation and signaling behavior of these cells determine follicular growth and hormone production. Cellular-level modeling has been applied using population dynamics and stochastic frameworks such as continuous-time Markov chains to capture the random events of cell division, death, and differentiation. Incorporating such cellular population models into higher-level follicle models provides a more mechanistic understanding of how cellular processes contribute to the overall dynamics of follicular maturation.



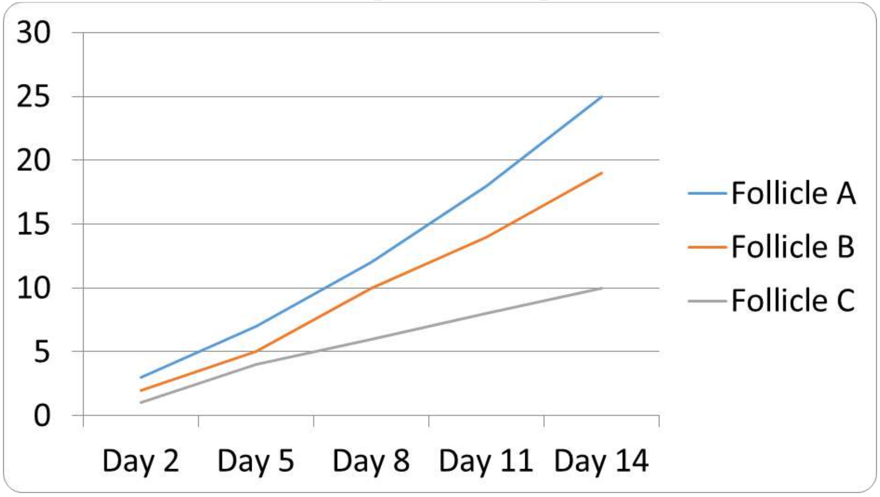
Stage-Based and Mass-Action Models

Another class of models defines follicular maturation in terms of discrete developmental stages; each associated with specific hormone-producing capabilities. Rather than focusing on the exact size or number of follicles, these models represent transitions between stages as state variables in a dynamical system. This abstraction allows the study of drug administration effects, follicular wave dynamics, and the impact of hormonal imbalances on ovulation. Such models have been particularly useful for exploring ovulatory dysfunctions and polycystic ovary syndrome, where disruptions in stage transitions can alter normal cycle progression.

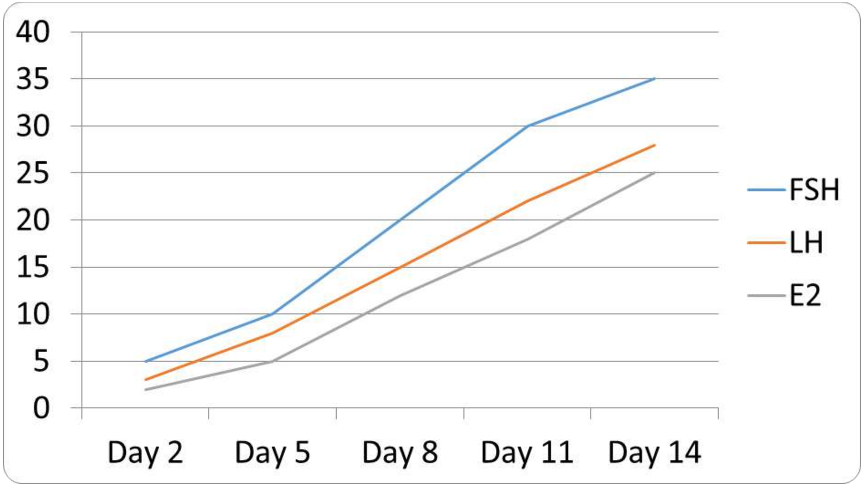
Follicle Population Models

Population-level models extend the analysis by simultaneously tracking the number and size of multiple follicles within a cycle. These models account for competition between follicles, in which the growth of one follicle can suppress the development of others. Extensions of these frameworks incorporate multiple ovulation events and allow coupling with hormonal regulation across the hypothalamic-pituitary-gonadal axis. By simulating the interplay between hormones and follicular maturation across consecutive cycles, such models can evaluate different stimulation protocols, predict ovarian responses, and provide a systems-level view of infertility treatment strategies.

Follicle Population Competition



Hormone Coupling: Hormones vs Follicle Growth



Treatment Computations and In-Silico Clinical Trials

Mathematical and mechanistic models provide a safe and efficient framework for predicting patient-specific outcomes in fertility treatments. These approaches form the foundation of in-silico clinical trials (ISCT), which can reduce the need for extensive laboratory experiments, animal studies, and early-stage human testing. By simulating physiological behaviors, these models enable clinicians to optimize individual treatment outcomes while minimizing risk.

Through parameter estimation and intelligent search strategies, large populations of virtual patients can be generated. Each virtual patient represents a unique set of physiological conditions, menstrual cycle dynamics, and responses to stimulation drugs. Such computational populations allow researchers to evaluate treatment protocols under diverse scenarios that would otherwise be impractical or ethically challenging to test in real life.

For example, virtual patient models can simulate the effect of different ovarian stimulation regimens, enabling the computation of personalized down-regulation protocols. These simulations help maximize the number of mature follicles and retrieved oocytes while simultaneously minimizing the likelihood of adverse side effects such as ovarian hyperstimulation. By integrating pharmacokinetic and pharmacodynamic components, these models can also test varying drug administration schemes, a task not easily addressed by purely statistical models.

The next phase of development lies in aligning these computational approaches with clinical practice. While the technological readiness of such methods is high, ethical and regulatory considerations must be carefully addressed before widespread adoption. Once integrated, in-silico trials have the potential to revolutionize reproductive endocrinology by making precision medicine a practical reality.

Conclusion

Mathematical modelling offers a powerful framework to study follicular dynamics, ovarian stimulation, and broader aspects of female reproductive health. Statistical models play a vital role in predicting the outcomes of in-vitro fertilization by analyzing patient and embryo characteristics, often supported by machine learning to identify the most influential factors.

On the other hand, mechanistic models provide deeper insights into the underlying biological and hormonal processes. They help to formulate and test hypotheses about complex system dynamics and identify critical parameters for experimental focus. Unlike statistical models, mechanistic frameworks can be directly coupled with pharmacokinetic simulations to evaluate drug administration strategies.

A particularly promising direction is the integration of mechanistic and machine learning approaches, where data-driven predictions are combined with theory-driven modeling to capture both observed and hidden dynamics. This hybrid approach enhances robustness and interpretability in clinical decision-making.

Future research is expected to merge statistical, mechanistic, and image-based models to provide a more holistic picture of reproductive processes. By doing so, mathematical modelling will continue to advance the field of infertility treatment, supporting precision medicine and improving outcomes for patients worldwide.

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Basics of Optical Chemosensor: Principle, Challenges and Mechanisms

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Abstract

Chemical sensors, or chemosensors, for detecting both negatively charged particles (anions) and positively charged particles (cations) have become indispensable across numerous fields, including pharmacology, environmental monitoring, biology, and chemistry. It focuses specifically on the design of systems that can identify and quantify these charged species by producing measurable signals, typically via optical (absorption or fluorescence properties) or electrochemical changes. The development of chemosensors remains an active and attractive area of research within supramolecular chemistry. This chapter specifically discuss the operational principles of chemosensor, the challenges inherent in their design and different mechanism by which chemosensor interact with the target analyte.

Keywords: Chemosensor, Optical Chemosensor, Anion and Cation detection, Internal Charge Transfer (ICT), Photoinduced Charge transfer (PET), Fluresscence Resonance Energy Transfer (FRET)

Introduction

Chemosensors

In the field of host guest chemistry, the term chemosensor is used for the interactions of molecular species between each other and the perturbation in its energy states. In general, the sensor is a system which can interact with the analyte and changes its own chemical or physical properties which provide valuable information that can be used to measure the analyte both by qualitatively as well as quantitatively. More specifically according to IUPAC guideline, a chemical sensor is device which can transform chemical information, ranging from concentration of a specific sample component to total composition analysis, into an analytically useful signal [1].The chemical sensors which transform information in the form of optical and photo-physical properties gains much more importance because such properties can be monitored by absorption, emission techniques which are easy to handle, highly sensitive, inexpensive and simpler.

Why Chemosensors Are Needed?

Ionic species has shown their widespread array in the field of catalysis, physiological processes, medical diagnostics, and environmental chemistry [2,3]. Anions in biological system carry genetic information (DNA as polyanion), enzyme substrates and co-factors are majorly anionic [4]. The ionic species (both cations as well as anions) are regnant in many fields like heavy industry, in farming, in the environment as pollutants, and their role well understood begin the use of chemical sensor to monitor their activities and concentrations. As per environmental concern, the cyanide (CN─) ions get more attention due to its highly toxic nature; it works damaging central nervous system [5]. It interacts at the active site of cytochrome a3, which inhibits the cellular respiration in mammalian cells [6]. The industries like petrochemical, gold mining, metal electroplating, photographic, steel manufacturing are major source of cyanide pollution [7]. Another anion fluoride (F─) has play important role in dental health [8] and useful in osteoporosis treatment [9]. It excreted from body at very slower rate while absorbed easily so it overexposure causes acute gastric and kidney problem [10]. In underdeveloped country, people get affected by drinking water causes debilitating bone disease fluorosis [11]. Aside from cyanide and fluoride, many other anions are involved in process of human body, environmental, industrial processes. Chloride ions are important for metabolism and to maintain ionic strength [12]. Bicarbonate, as important constituent of pH buffering system inside of the body, regulates the physiological pH [13]. Phosphate anions are indispensible part of ATP and ADP, involved in energy transfer and signal transport [14]. Excessive use of phosphate and nitrates rich fertilizers in agriculture causes eutrophication due to its contamination in aquatic system [15]; nitrate and sulphate are the major content of acid rain [16]. The radioactive pertechnetate ions, the wastage of nuclear fuel processing industries causes a serious pollution to human health [17]. As like anions, the cations are also important part of natural processes like in plant the light energy production by photosynthesis is rely on magnesium (II) (Mg2+) present in chlorophyll; ferrous ion (Fe2+) present in haemoglobin is important for respiration [18]; sodium (Na+) and potassium (K+) are suited for generating ionic gradients across the membrane and vital for maintaining osmotic balance [19]. Cobalt is essential element for coenzyme B12 and believed to be cardiotoxic and responsible for lung damage. The copper (II) is essential for iron absorption, haemopoiesis, number of enzymes catalysed and redox reactions in biological processes [20]. Apart from biological importance the cations are important in medicinal, environmental processes and for other applications. The silver(I) (Ag+) used to inhibit bacterial and fungal growth to prevent its infection and also useful in radio-immunotherapy, cloth deodoriser and agricultural sterilizing agents [21]. The mercury is one of the highly poisonous elements in the periodic table. It leads to serious environmental and health problems. Its exposure even at lower concentration leads to damage to digestive, kidney, and more importantly neurological systems. Coal and gold mining, solid waste incinerations, wood pulping, combustion of fossil fuel, chemical industries are the major sources of mercury [22]. Vapour form of mercury can easily be transported in atmosphere, may cross continents and ocean, and sometimes get oxidized to Hg (II) [23]. United State Environmental Protection Agency (EPA) has approved maximum 2 ppb (10 nM) for Hg (II) in drinking water system [24].

Hence, from above discussion as the ions plays vital role in biological systems, environmental systems, and in numerous chemical processes, the importance of designing and synthesising host receptors for ionic species cannot be overstated. The next section includes the detailed discussion about challenges for ions sensing, instrumental techniques and principles of ions sensing.

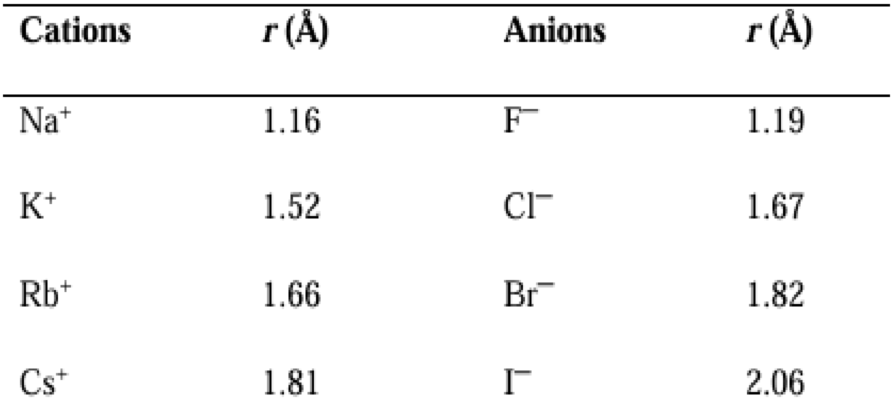
Challenges In Anion Recognition

The anions are possessing certain inherent properties which are need to consider while designing the chemical receptors. Because of these properties the field of anion sensor grow slower as compared to that of cations.

1. Size of Anion

The anions have larger size as compared with its isoelectronic cations (Table 1) [25] which decreases charge to radius ratio. Therefore, it decreases the electrostatic interaction of anions with host receptor as compared to cations.

Table 1. The comparison of ionic radii in (Å) of anions with their isoelectronic cation in octahedral environment.



Cations	*r* (Å)	Anions	*r* (Å)
Na^+	1.16	F^-	1.19
K^+	1.52	Cl^-	1.67
Rb^+	1.66	Br^-	1.82
Cs^+	1.81	I^-	2.06

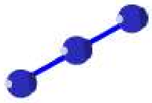
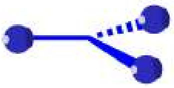
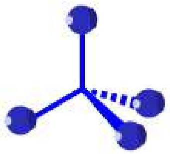
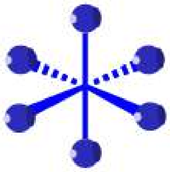
2. pH Value

Certain anions are more sensitive to the pH value as they readily get protonated at lower pH value and lose their negative charge like carboxylate (RCOO─) ions are get easily protonated at highly acidic pH. In certain cases, host receptor system themselves pH sensitive like polyammonium system are get deprotonated at higher pH value makes ineffective for anions recognition at higher pH value.

3. Geometry

Anions are present in wide variety of shapes and geometries, like spherical (halides), linear (azide, cyanide, hydroxyl), Trigonal planar (carbonate, nitrate), tetrahedral (sulfate, perchlorate), octahedral (hexafluorophosphate) (Table 2); demands to design the receptor with complementary binding site for selective recognition. So as compared with cations (most of them are spherical), designing of anion receptor is more challenging task.

Table 2. Different geometries of anions.

	Spherical	F^-, Cl^-, Br^-, I^-
	Linear	N_3^-, CN^-, OH^-
	Trigonal planar	CO_3^-, NO_3^-
	Tetrahedral	SO_4^-, ClO_4^-
	Octahedral	PF_6^-

4. Solvent Effect

Solvent plays a crucial role in anion complexation. As the anions can easily get solvated compared with its isoelectronic cations [26, 27], the host receptor for anions must compete with the solvent environment effectively to get strong and selective anion binding in aqueous media is a significant challenge.

5. Hydrophobicity

The selectivity for anion recognition is affected by the hydrophobicity of anions. The Hofmeister series (Figure 1. [28], based on the effect of salts on the solubility of protein, orders the anions according to hydrophobicity of anions (and degree of solvation), to design selective receptor for anion which can effectively compete with solvent.

Organic anions > ClO_4^- > SCN^- > I^- > salicylate > NO_3^- > Br^- > Cl^- > HCO_3^- > $H2PO_4^-$ > F^- ≈ SO_4^{2-}> HPO_4^{2-}

Figure 1. The Hofmeister series.

Molecular Recognition System

Generally, molecular recognition system i.e. chemical sensor is made up of two constituents namely binding sites and signalling unit (or transducer) (Figure 2.). The binding site of receptor interacts/binds with analytes and signalling unit convert these interactions of analyte with receptor into a measurable physical change which can be monitored through different analytical techniques. The interaction of analyte with receptor can be monitored through different analytical techniques viz. absorption and/or fluorescence (optical sensor), cyclic voltammetry (electrochemical sensor) etc. Apart from these properties, the thermal [29], mechanical [30], electrical [29] are also useful to generate output signal.

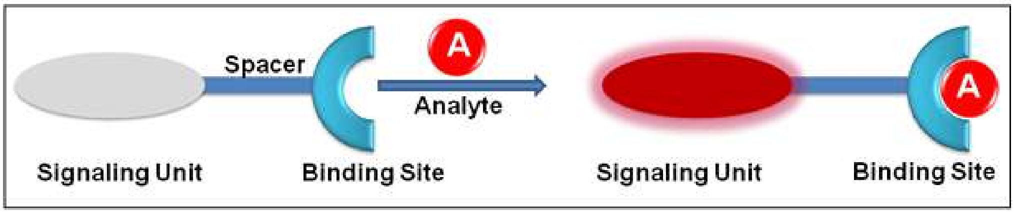


Figure 2. Schematic representation of chemical sensor system.

The interactions of analytes with receptor are of three different types namely
(a) Binding site-signaling approach, (b) Displacement approach,
(c) Chemodosimetric approach

Binding Site-Signaling Approach

Binding site-signaling approach is same as presented in Figure 1.2; comprises of binding site and signaling unit are connected with covalent bonds. The analyte interacts with the binding sites with different kinds of interaction viz. Van der Waals forces, hydrogen bonding interactions and electrostatic interactions [31]; and perturbs electronic properties of signaling unit which is utilized for sensing of targeted ion.

Displacement Approach

In the displacement approach the signaling unit and binding site are ensemble system (i.e molecular assembly). When targeted analyte added to the solution of signaling unit and binding site system, follows displacement reaction. The analyte coordinates with binding site and release the signaling unit (or indicator) into the solution bearing its noncoordinated spectroscopic properties [32] (Figure 3). This approach is helpful when the stability constant for the formation of complex between binding site and analyte is higher than that between binding site and signaling unit.

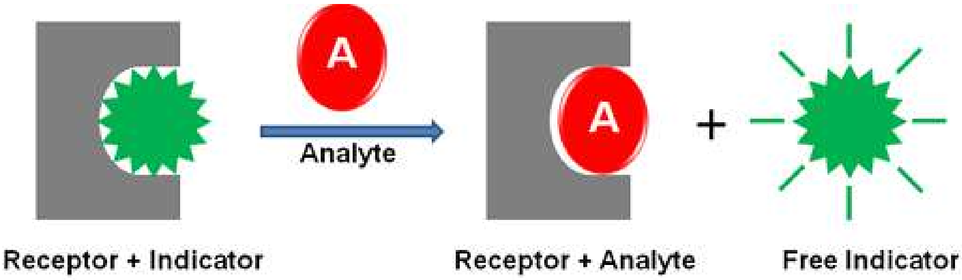


***Figure 3. Displacement apprach for chemosensor*.**

Chemodosimetric Approach

In chemosdosimetric aproach, the targeted analyte induced chemical reaction occurs to form a product with different optical properties. Figure 4 represents the two types of chemodosimetric approach, in first case the analyte froms covalent or coordinate bonded product with chemodosimeter; and in second case, analyte induced chemical reaction occured to form a product. In both the cases, the optical properties of final product are different than starting material allows recognition of targeted analyte [33]. The advantage of chemodosimetric approach is that the reaction is very specific with particular analyte so the system provides high selectivity.

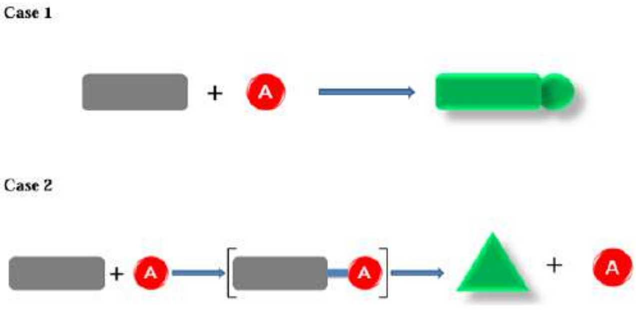


Figure 4. Chemodosimetric approach for molecular recognition system.

The Photophysics of Optical Sensor

The optical chemosensors can be divided into two categories

a. **Chromogenic Chemosensor:** When interaction of binding site of a receptor or chemosensor with analytes is associated with colour change of signaling unit can be reffered as chromogenic chemeosensor.
b. **Fluorogenic Chemosensors:** When the interaction of binding site of receptor or chemosensor with analyte is associatd with changes in fluorescence properties of the system referred as fluorogenic chemosnsor.

The response of the chemosensor after interaction with targeted analyte is controlled by different mechnisms viz. Internal Charge Transfer (ICT), Photoinduced Charge transfer (PET), Flurescence Resonance Energy Transfer (FRET), Metal to Ligand Charge Tranfer (MLCT) etc.

1. Internal Charge Transfer

Excitation of electron is required to occure some degree of charge transfer process in the molecular system. In typical internal charge transfer (ICT), system comprises of electron donor (D) and electron acceptor (A) substituents; and both are linked through conjugated system (π- system). The dipole moment of system is differed in both ground and excited electronic state. The system upon electronic excitation, the internal charge gets transferred from donor site to acceptor site through conjugation and produce internal charge transfer (ICT) process [34].

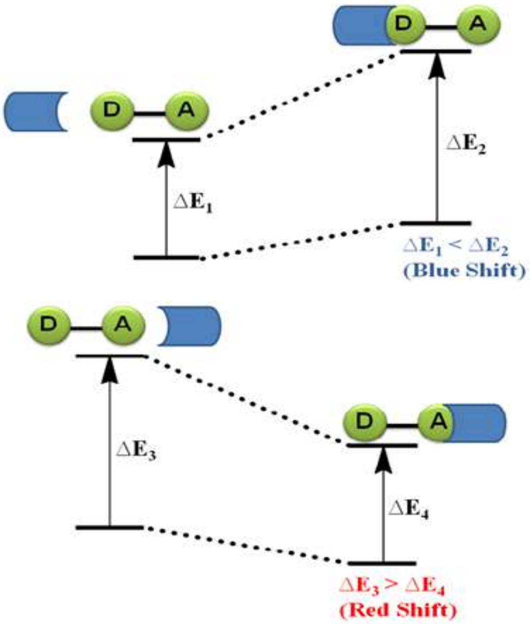


Figure 5. Internal Charge Tranfer (ICT) process; interaction of analyte with (a) donor and (b) acceptor site.

The ICT process is highly sensitive to its mocroenvironment of the system. The interaction of analyte with either donor or acceptor site is associated with the changes in photophysical properites of the system. When analyte binds to the electron donor site of the system, the electron donation character of donor site will reduce, results in reduction of charge transfer causes the blue shift in absorption spectra and lowers the molar absorptivity (Figure 5a). On the other hand, when analyte intearact at the acceptor site, it will enhance the resultant charge transfer from donor to acceptor site, and reduce the energy required for excitation (Figure 5b). Such system shows red shift in absorption spectra and also increases in molar absorptivity. The absorption spectral behavior is aligned in emission spectra of the system. Along with these, the changes in quantum yield and life time can also be oberved in some cases.

2. Photoinduced Electron Transfer (PET)

The photoinduced electron transfer mechanism is largely studied and used for recognition of both cations and anions. Typically, fluorescence is observed when excited state electron of fluorophore from lowest unoccupied molecular orbital (LUMO) goes to the highest occupied molecular orbital (HOMO) by releasing energy in the form of light. In certain case, another part of the system may have the its orbital with energy in between that of HOMO and LUMO of the fluorophore. When such alien orbitals have electron pair, then PET mechanism followed from this electron fulled orbital to the HOMO orbital of fluorophore and the excited electron from the LUMO of fluorophore will come to the external orbital retieves ground state (Figure 6a) [34]. As a result of these processes, the system follows non-radiative relaxation pathways and the system becomes non-fluorescent. There is another condition for PET mechanism is that if the vacant orbital of another part of system appear in between HOMO and LUMO of fluorophore energy level, then electron from excited state LUMO orbital get transferred in vacant orbital followed by transfer of electron from this orbital to ground state HOMO orbital of the fluorophore. In this way the quenching of fluorescence occurs through this mechanism. The advantage of such system is useful to design chemosensor for detection of analyte (anions or cations), like presence of analyte can make the appearance or removal of energy level in between HOMO and LUMO of the system which causes either quenching or increase of fluorescence (Figure 6b).

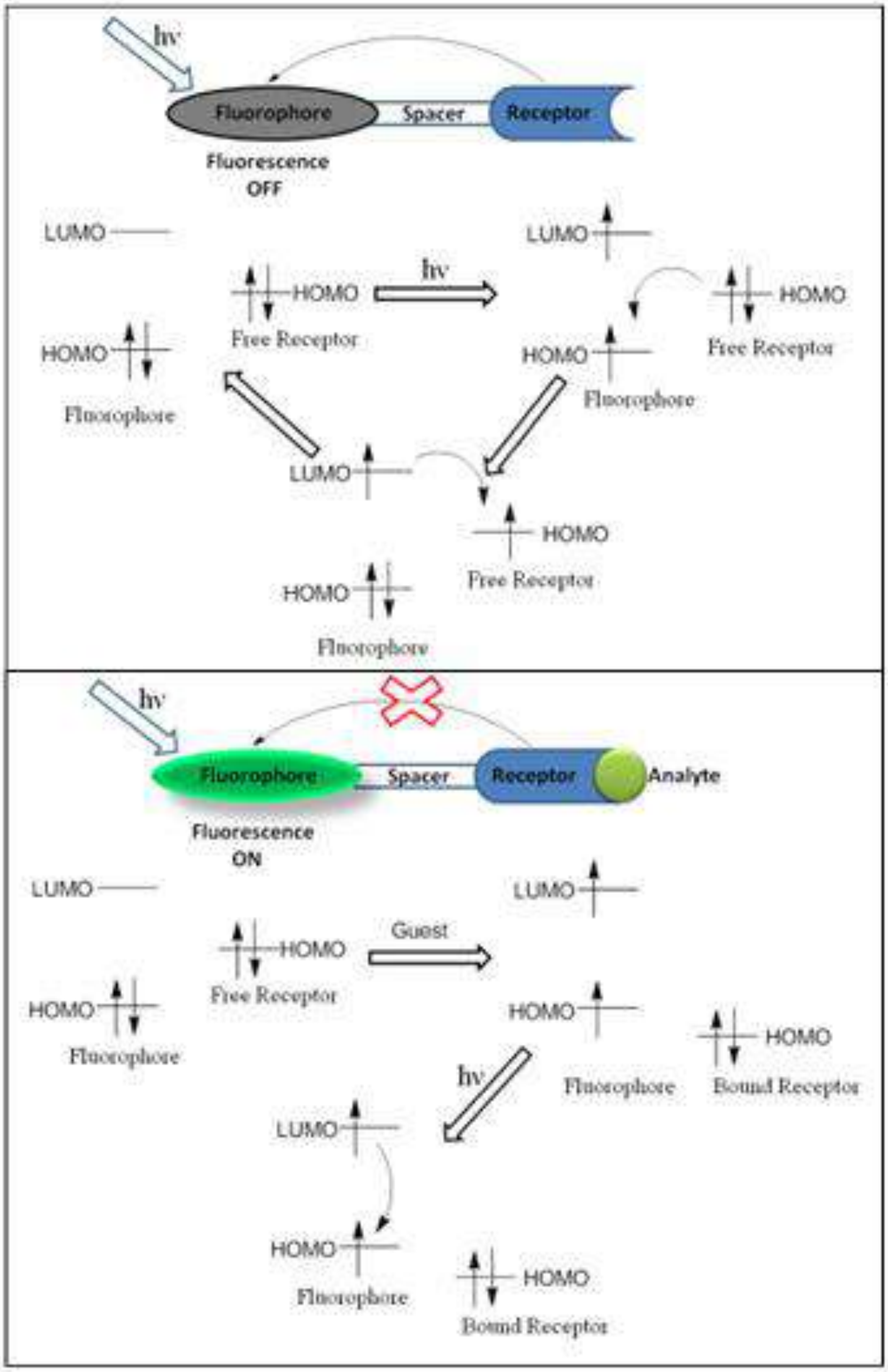


Figure 6. Photoinduced Energy Transfer (PET) mechanism; a) without analyte and b) with analyte.

3. Flurescence Resonance Energy Transfer (FRET)

FRET is another important mechanism used for detection of analyte. It is an interaction of electronically excited state of one fluorophore and another fluorophore within the molecule where the excitation is transferred from donor site to acceptor site with no emission, and when the FRET is in ON state another site of fluorohore gives emission [35]. There are certain certain points that need to be consitder while designing FRET based sensor;

- donor and acceptor site should be closer around 10-100 Å
- the emission spectra of donor must overlap with absorption spectra of acceptor site
- the orientation of donor and acceptor transition dipole should be parellal.

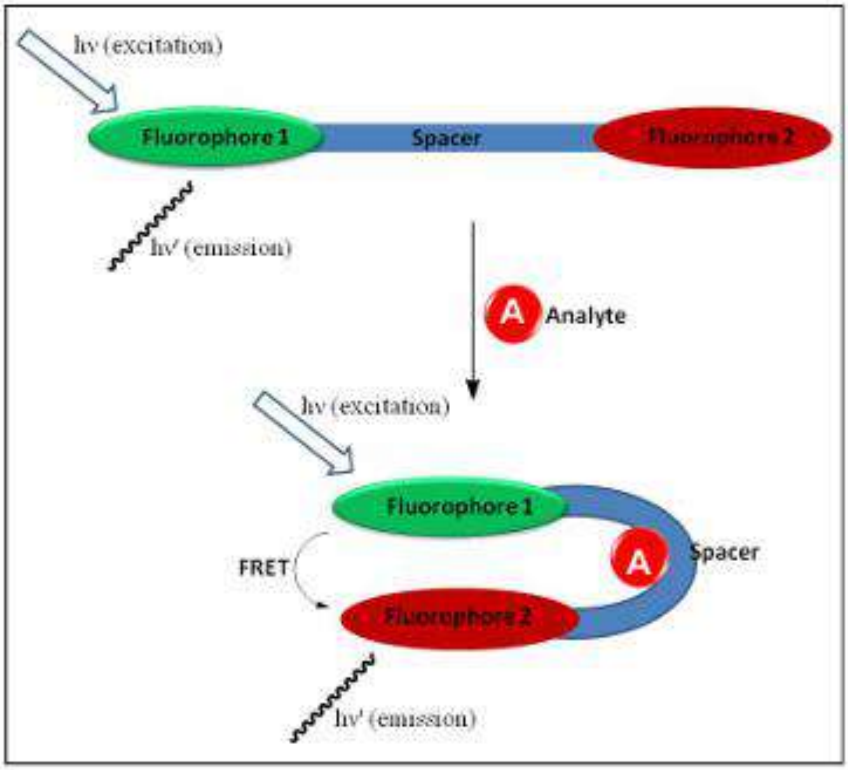


Figure 7. FRET mechanism representations.

The presence of analyte can monitor the orientation of the two fluorophore and useful for recognition. As shown in Figure 7, the excitation of fluorophore-1 give emission out without FRET mechnism as both the fluorophores are on great distant. Due to interaction of analyte the two-fluorophore come in close porximity make FRET in ON state, thus excitation of fluorophore-1 gives emission of fluorophore-2 can detected.

4. Metal to Ligand Charge Transfer (MLCT)

The chemosensor incorporated with transition metal provide another class of recognition mechanism. As the transition metal complexes are well known for their long-lived metal to ligand charge (MLCT) transition, compared to traditional organic chemosensors. Specially, Ruthenium (II), Osmium (II), Rhenium(I) metal complexes show highly sensitive MLCT band around 450 nm (in visible region), this band is highly sensitive microenvironment i.e. upon interaction of analyte with ligand site gives perturbation in energy level of MLCT band which can monitored by colour change simply.

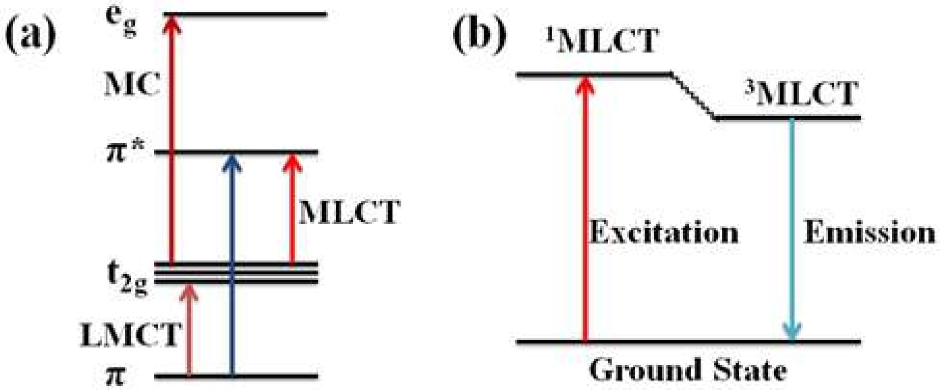


Figure 8. Molecular Orbital and Jablonski diagram for Ruthenium (II) metal complexes.

For example, octahedral Ruthenium (II) metal complex have low spin d6 electronic configuration with molecular energy diagram as in Figure 8a. The metal complexes show number of electronic transitions like metal centred d-d transition, ligand centred π-π* transitions, LMCT (ligand to metal charge transfer) and MLCT (metal to ligand charge transfer). This last MLCT band is plays crucial role in terms of photophysical properties of the complexes, by absorption of light electron get excited from fully filled t2g orbital of Ru (II) metal to ligand centred π* energy orbital. The intersystem crossing (ISC) from 1MLCT state to 3MLCT state occurred and comes to the round state with strong emission (Figure 8b). The interaction of analyte perturbs the MLCT band transitions provide helpful tool to monitor the system for molecular recognition. Apart from these mechanisms, interaction of analyte with chemosensors can also follow different mechanism, like Excited State Intramolecular Proton Transfer (ESIPT), Aggregation Induced Emission (AIE), Twisted Intramolecular Charge Transfer (TICT), Chelation Enhanced Fluorescence effect (CHEF) or Chelation Enhanced Quenching effect (CHEQ) etc.

Conclusion

Overall, optical chemosensors are promising tools for the detection of anions and cations across various applications, including the pharmaceutical, environmental, and food industries, indicating broad utility and promising future directions. The chapter highlighted critical design challenges that must be considered when developing new chemosensors, such as ionic size, geometry, solvent effects, pH, and hydrophobicity. Furthermore, a clear understanding of the different types of interaction mechanisms between the chemosensor and targeted ions, which are responsible for changes in absorption and/or fluorescence properties, was discussed.

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Finite Differences

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Abstract

Finite differences are essential for approximating derivatives and solving numerical problems in calculus, particularly in interpolation and differential equations. This chapter outlines three fundamental types: forward, backward, and central differences, each with its respective operators and formulas. Forward differences estimate function changes moving forward, while backward differences track changes in reverse. Central differences, measured around a midpoint, enhance numerical accuracy. Key difference operators, including the shift operator E and averaging operator μ, are introduced with their interrelations.

Key Words: Finite Differences, Tools, Computational Mathematics

1. Introduction

Finite differences are fundamental mathematical tools used to approximate derivatives and analyze numerical data. They are widely applied in numerical analysis, particularly in solving differential equations, interpolation, and numerical differentiation. When a function is known only at discrete points, finite differences help estimate function values and their derivatives at other points.

This method is especially useful in computational mathematics, where exact differentiation may not be possible. Instead of using continuous functions, finite difference techniques rely on discrete values, making them ideal for applications such as physics, engineering, and computer simulations.

In this study, we explore the different types of finite differences:

- **Forward Differences:** Used to compute changes in function values in a forward manner.

- **Backward Differences:** Measures changes by considering values moving backward in a sequence.
- **Central Differences:** Provides a more balanced approximation by computing differences symmetrically around a point.

  Along with these, we discuss difference tables, operators, and their relations, along with practical examples to illustrate the use of finite differences in polynomial calculations and numerical differentiation.

1.1 Finite Differences:

Suppose we have a function y=f(x) that is given in a table, with values of x spaced equally as $x = x_0$, $x_0 + h$, $x_0 + 2h$,…,$x_0 + nh$ corresponding to function values $y = y_0$,y_1 ,y_2 ,…,y_n . To estimate the value of f(x) or its derivative f′(x) at a point x that falls between these tabulated values, we can use numerical methods such as interpolation for the function value and finite differences for the derivative, the following three types of differences are found useful:

1.1.1) Forward differences:

- **First Forward Difference:**

  The difference between two consecutive values of y is called the first forward difference. It is given by:

$$\Delta\, y_r = y_{r+1} - y_r$$

This helps us see how the values change step by step.

- **Second Forward Difference:**

  The difference between two consecutive first differences is called the second forward difference:

$$\Delta^2 y_r = \Delta y_{r+1} - \Delta y_r$$

This tells us how the change itself is changing.

- **General Forward Difference (p-th order):**

  Higher-order differences follow the pattern:

$$\Delta^p y_r = \Delta^{p-1} y_{r+1} - \Delta^{p-1} y_r$$

Each step compares the previous level of differences.

❖ Difference Table Structure:

- The values of x are called arguments.
- The values of y are called entries or the function values.
- The first value of y (y_0) is called the initial term.
- The differences $\Delta y_0, \Delta^2 y_0, \Delta^3 y_0, \ldots$ are called the initial differences.

Forward Difference Table

V Value of	V Value of y	1st Diff.	2nd Diff.	3rd Dif	4th Diff.	5th Diff
x_0	y_0					
		Δy_0				
$x_0 + h$	y_1		$\Delta^2 y_0$			
		Δy_1		$\Delta^3 y_0$		
$x_0 + 2h$	y_2		$\Delta^2 y_1$		$\Delta^4 y_0$	
		Δy_2		$\Delta^3 y_1$		$\Delta^5 y_0$
$x_0 + 3h$	y_3		$\Delta^2 y_2$		$\Delta^4 y_1$	
		Δy_3		$\Delta^3 y_2$		
$x_0 + 4h$	y_4		$\Delta^2 y_3$			
		Δy_4				
$x_0 + 5h$	y_5					

1.1.2 Backward differences:

- **First Backward Difference (∇y)**

The first backward difference measures the difference between a value and the one before it:

$$\nabla y_r = y_r - y_{r-1}$$

This tells us how much the function is changing when moving backward in the table.

- **Second Backward Difference ($\nabla^2 y$)**

The second backward difference is the difference between two consecutive first backward differences:

$$\nabla^2 y_r = \nabla y_r - \nabla y_{r-1}$$

This shows how the rate of change itself is changing.

- **Higher-Order Backward Differences($\nabla^p y$)**

We can continue this pattern to find higher-order differences:

$$\nabla^3 y_r=\nabla^2 yr-\nabla^2 y_{r-1}$$

$$\nabla^p y_r=\nabla^{p-1} y_r-\nabla^{p-1} y_{r-1}$$

Each step compares the previous level of differences.

Backward Difference Table

V Value of x	V Value of y	1st Diff.	2nd Diff.	3rd Diff.	4th Diff.	5th Diff.
x_0	y_0					
		∇y_1				
$x_0 + h$	y_1		$\nabla^2 y_2$			
		∇y_2		$\nabla^3 y_3$		
$x_0 + 2h$	y_2		$\nabla^2 y_3$		$\nabla^4 y_4$	
		∇y_3		$\nabla^3 y_4$		$\nabla^5 y_5$
$x_0 + 3h$	y_3		$\nabla^2 y_4$		$\nabla^4 y_5$	
		∇y_4		$\nabla^3 y_5$		
$x_0 + 4h$	y_4		$\nabla^2 y_5$			
		∇y_5				
$x_0 + 5h$	y_5					

1.1.3) Central differences:

Sometimes, it is useful to use a different type of difference system called central differences. Instead of comparing values in a forward or backward manner, central differences measure changes around a central point.

• Definition of the Central Difference Operator (δ)

The central difference operator (δ\deltaδ) is defined as:

$$y_1 - y_0 = \delta y_{1/2},\ y_2 - y_1 = \delta y_{3/2},\ \ldots,\ y_n - y_{n-1} = \delta y_{n-\frac{1}{2}.},$$

This means that each central difference represents the change between two neighbouring function values but is assigned to the midpoint of the interval.

- Higher-Order Central Differences

Just like forward and backward differences, we can extend central differences to higher orders:

$$\delta y_{5/2} - \delta y_{3/2} = \delta^2 y_2$$

$$\delta^2 y_2 - \delta^2 y_1 = \delta^3 y_{3/2}$$

And so on. Each new difference level is found by subtracting the previous difference values. These differences are shown in Table.

Central Difference Table

And so on. Each new difference level is found by subtracting the previous difference values. These differences are shown in Table.

V Value of x	V Value of y	1 1st Diff.	2nd Diff.	3rd Diff.	4th Diff.	5th Diff.
x_0	y_0					
		$\delta y_{1/2}$				
$x_0 + h$	y_1		$\delta^2 y_1$			
		$\delta y_{3/2}$		$\delta^3 y_{3/2}$		
$x_0 + 2h$	y_2		$\delta^2 y_2$		$\delta^4 y_2$	
		$\delta y_{5/2}$		$\delta^3 y_{5/2}$		$\delta^5 y_{5/2}$
$x_0 + 3h$	y_3		$\delta^2 y_3$		$\delta^4 y_3$	
		$\delta y_{7/2}$		$\delta^3 y_{7/2}$		
$x_0 + 4h$	y_4		$\delta^2 y_4$			
		$\delta y_{5/2}$				
$x_0 + 5h$	y_5					

- **Observations from the Central Difference Table**

1. Same Suffix for Central Differences on the Same Line:

All central differences at the same horizontal level have the same subscript.

2. Odd-Order Differences Appear at Half-Values:

Differences of the first, third, and other odd orders are assigned to midpoints (fractions like 1/2 ,3/2 etc.).

3. Even-Order Differences Are at Whole Numbers:

Differences of the second, fourth, and other even orders are assigned to whole number positions (1, 2, etc.).

It is often required to find the mean of adjacent values in the same column of differences. We denote this mean by μ.

Thus $\mu\delta y_1 = \frac{1}{2}\left(\delta y_{\frac{1}{2}} + \delta y_{\frac{3}{2}}\right)$, $\delta^2 y_{\frac{3}{2}} = \frac{1}{2}\ (\delta^2 y_1 + \delta^2 y_2\ )$, etc.

Worked Examples:

Example 1: $\Delta \tan^{-1}x$

Solution:

$$\Delta \tan^{-1}x = \tan^{-1}(x+h) - \tan^{-1}x$$

$$= \tan^{-1}\{\frac{x+h-x}{1+(x+h)x}\}$$

$$\Delta \tan^{-1}x = \tan^{-1}\{\frac{h}{1+x^2+hx}\}$$

Example 2: $\Delta(e^x \log 2x)$

Solution:

$$\Delta\ (e^x \log 2x) = e^{x+h}\ log2(x+h) - e^x log2x$$

$$= e^{x+h}\ log2(x+h) - e^{x+h}\ log2x + e^{x+h}\ log2x - e^x log2x$$

$$= e^{x+h}\ log\frac{x+h}{x}\ (e^{x+h}\ - e^x)log2x$$

$$= e^x[e^h \log\left(1+\frac{h}{x}\right) + (e^h - 1)log2x\ ]$$

1.2 Differences of a Polynomial:

The nth differences of a polynomial of the nth degree are constant and all higher order differences are zero.

Let the polynomial of the nth degree in x, be

$$f(x) = ax^n + bx^{n-1} + cx^{n-2} + \ldots + kx + l$$

$$\therefore\ \Delta f(x) = f(x+h) - f(x)$$

$$= a[(x+h)^n - x^n] + b[(x+h)^{n-1} - x^{n-1}] + \ldots + kh$$

$$= anhx^{n-1} + b'x^{n-2} + c'x^{n-3} + \ldots + k'x + l' \quad \text{- - - - (1)}$$

where b′, c′, …,l′ are the new constant co–efficient.

Thus, the first differences of a polynomial of the nth degree is a polynomial of degree (n – 1).

Similarly,

$$\begin{aligned}\Delta^2 f(x) &= \Delta[f(x+h) - f(x)]\\ &= \Delta f(x+h) - \Delta f(x)\\ &= anh[(x+h)^{n-1} - x^{n-1}] + b'[(x+h)^{n-2} - x^{n-2}] + \ldots + k'h\\ &= an(n-1)h^2 x^{n-2} + b''x^{n-3} + c''x^{n-4} + \ldots + k'' \text{ - - - - by (1)}\end{aligned}$$

∴ The second differences represent a polynomial of degree (n – 2).

Continuing this process, for the nth differences we get a polynomial of degree zero i.e.

$$\Delta^n f(x) = an(n-1)(n-2)\ldots1.h^n = an\,!h^n \qquad \text{- - - - - - - (2)}$$

Which is a constant. Hence the (n + 1)th and higher differences of a polynomial of nth degree will be zero.

Worked Examples:

Example 1: Evaluate: $\Delta^{10}[(1-ax)(1-bx^2)(1-cx^3)(1-cx^3)(1-dx^4)]$.

Solution: $\therefore\Delta^{10}[(1-ax)(1-bx^2)(1-cx^3)(1-dx^4)]$

$$\begin{aligned}&= \Delta^{10}[abcd\ x^{10} + (\ )x^9 + (\ )x^8 + \ldots + 1]\\ &= abcd\,\Delta^{10}(x^{10}) \qquad [\therefore\ \Delta^{10}(x^n) = 0 \text{ for } n<10]\\ &= abcd(10!) \qquad [\text{by (2) above}]\end{aligned}$$

1.3 Other Difference Operators

We have already introduced the operators Δ, Δ, and δ. Besides these, there are the

operators E and μ, which we define below:

Shift operator E is the operation of increasing the argument x by h

so that $Ef(x) = f(x+h)$, $E^2f(x) = f(x+2h)$, $E^3f(x) = f(x+3h)$ etc.

The inverse operator $E^{-1}$is defined by $E^{-1}f(x) = f(x-h)$.

If y_x is the function f(x), then

$Ey_x = y_{x+h}$,

$E^{-1}y_x = y_{x-h}$

$E^n\, y_x = y_{x+nh}$, where n may be any real number. Averaging operator **μ** is defined by the equation,

$$My_x = \frac{1}{2}\left(y_{x+\frac{1}{2}h} + y_{x-\frac{1}{2}h}\right)$$

Relations Between the Operators:

We shall now establish the following identities:

1) $\Delta = E - 1$

2) $\Delta = 1 - E^{-1}$

3) $\delta = E^{1/2} - E^{-1/2}$

4) $\mu = \frac{1}{2}(E^{\frac{1}{2}} - E^{-\frac{1}{2}})$

5) $\Delta = E\Delta = \Delta E = \delta E^{1/2}$

6) $E = e^{hD}$.

Proofs:

(i) $\Delta y_x = y_{x+h} - y_x$

$= Ey_x - y_x$

$= (E-1)y_x$.

This shows that the operators Δ and E are connected by the symbolic relation.

$\Delta = E - 1$ or $E = 1 + \Delta$.

(ii) $\Delta y_x = y_x - y_{x-h}$

$= y_x - E^{-1}y_x$

$\Delta y_x = (1 - E^{-1})y_x$

$\therefore \Delta = 1 - E^{-1}$

(iii) $\delta\, y_x = y_{x+\frac{1}{2}h} + y_{x-\frac{1}{2}h}$

$= E^{1/2}\ y_x - E^{-1/2} y_x$

$= (E^{1/2} - E^{-1/2})\ y_x$

$\therefore\ \delta = E^{1/2} - E^{-1/2}$

(iv) $\mu y_x = \frac{1}{2}(y_{x+\frac{1}{2}h} + y_{x-\frac{1}{2}h})$

$= \frac{1}{2}(E^{\frac{1}{2}}\ y_x - E^{-\frac{1}{2}}\ y_x)$

$= \frac{1}{2}(E^{\frac{1}{2}} - E^{-\frac{1}{2}})y_x$

$\therefore\ \mu = \frac{1}{2}(E^{\frac{1}{2}} - E^{-\frac{1}{2}})$

(v) $E\Delta\ y_x = E(y_x - y_{x-h})$

$= Ey_x - Ey_{x-h}$

$= y_{x+h} - Ey_x$

$= \Delta y_x$

$\therefore\ E\ \Delta = \Delta$

$\Delta E y_x = \Delta y_{x+h}$

$= y_{x+h} - y_x$

$= \Delta y_x$

$\therefore\ \Delta E = \Delta$

$\delta E^{1/2}\ y_x = \delta y_{x+\frac{1}{2}h}\ \frac{1}{2}h - y_{x+\frac{1}{2}h} - \frac{1}{2}h - \frac{1}{2}h$

$= y_{x+h} - Ey_x$

$= \Delta y_x$

$\therefore\ \delta E^{1/2} = \Delta$

Hence, $\Delta = E\Delta = \Delta E = \delta E^{1/2}$

(vi) $Ef(x) = f(x+h)$

$$= f(x)+hf'(x)+\frac{h^2}{2!}f''(x)+\ldots\ldots$$

- - - -[By Taylors series]

$$= f(x)+hDf(x)+\frac{h^2}{2!}D2\ f(x)+\ldots\ldots$$

$$= \left(1+hD+\frac{h^2}{2!}+\frac{h^3}{3!}+\cdots\right)f(x)$$

$$= e^{hD}f(x)$$

$$\therefore\ E = e^{hD}f(x)$$

Relations between the various operators

In terms of	E	Δ	∇	δ	hD
E	---	$1+\Delta$	$(1-\nabla)^{-1}$	$1+\frac{1}{2}\delta^2+\Delta\sqrt{1+\delta^2/4}$	e^{hD}
Δ	$E-1$	---	$(1-\nabla)^{-1}-1$	$\frac{1}{2}\delta^2+\Delta\sqrt{1+\delta^2}$	$e^{hD}-1$
∇	$1-E^{-1}$	$1-(1+\Delta)^{-}$	---	$-\frac{1}{2}\delta^2+\Delta\sqrt{1+\Delta^2/4}$	$1-e^{-hD}$
σ	$E^{1/2}-E^{-1/2}$	$\Delta(1+\Delta)^{-1/}$	$\Delta(1-\Delta)$	---	sinh (hD/2)
δ	$\frac{1}{2}(E^{1/2}-E^{-1/}$	$(1+\Delta/2)(1+\Delta)^{-1/2}$	$(1+\Delta/2)(1-\Delta)^{-1/}$	$\sqrt{1+\Delta^2/4}$	cosh(hD/2)
hD	logE	$\log(1+\Delta)$	$\log(1-\nabla)^{-1}$	2sinh-1 (δ/2)	---

Worked Examples:

Example 1: Prove with the usual notations, that

$$hD = \log(1+\Delta) = -\log(1-\nabla) = \sin^{-1}(\mu\delta)$$

Solution:

We know that, $e^{hD} = E = 1+\Delta$

$$\therefore \mathrm{hD} = \log(1+\Delta)$$

Also, $hD = logE = -\log(E^{-1}) = -\log(1-\nabla)$

- - -[E^{-1}=1- ▽]

We have proven that,

$$\mu = \frac{1}{2}(E^{\frac{1}{2}} + E^{-\frac{1}{2}})$$

and $$\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}}$$

$$\mu\delta = \frac{1}{2}(E^{\frac{1}{2}} + E^{-\frac{1}{2}})(E^{\frac{1}{2}} - E^{-\frac{1}{2}})$$

$$= \frac{1}{2}(E - E^{-1})$$

$$= \frac{1}{2}(e^{hD} - e^{-hD})$$

$$= \sinh(hD)$$

$$hD = Sinh^{-1}(\mu\delta)$$

Hence

$$\therefore hD = \log(1+\Delta) = -\log(1-\nabla) = \sin^{-1}(\mu\delta)$$

Example 2: Prove that, $\Delta = \frac{1}{2}\delta^2 + \delta\sqrt{(1+\frac{\delta^2}{4})}$

Solution:

$$\frac{1}{2}\delta^2 + \delta\sqrt{(1+\frac{\delta^2}{4})}$$

$$= \frac{1}{2}\left(E^{\frac{1}{2}} - E^{-\frac{1}{2}}\right)^2 + \left(E^{\frac{1}{2}} - E^{-\frac{1}{2}}\right)\sqrt{[1 + \left(E^{\frac{1}{2}} - E^{-\frac{1}{2}}\right)^{2/4}]}$$

$$= \frac{1}{2}(E + E^{-1} - 2) + \left(E^{\frac{1}{2}} - E^{-\frac{1}{2}}\right)\sqrt{\frac{E+E^{-1}+2}{4}}$$

$$= (E + E^{-1} - 2) + \left(E^{\frac{1}{2}} - E^{-\frac{1}{2}}\right)\left(E^{\frac{1}{2}} + E^{-\frac{1}{2}}\right)/2$$

$$= \frac{1}{2}[(E + E^{-1} - 2) + (E - E^{-1})$$

$$= E-1$$

$$\therefore \frac{1}{2}\delta^2 + \delta\sqrt{(1+\frac{\delta^2}{4})} = \Delta$$

Example 3: Find the value of E^2x^2 when the values of x vary by a constant increment of 2.

Solution: We have,

$$\begin{aligned} E^2x^2 &= E\,E\,x^2 \\ &= E(x+2)^2 \qquad [\because \text{ interval of differencing is } 2\ ] \\ &= (x+2+2)^2 \\ &= (x+4)^2 \\ &= x^2 + 8x + 16 \end{aligned}$$

Conclusion

The nth difference of a polynomial of degree n is constant, with higher-order differences becoming zero. In this chapter, author has explained forward, backward, and central differences, each with its respective operators and formulas. He also showed the inter relations between different operators used for finite differences and solved some examples to illustrate these principles, showing their applications in evaluating finite differences of functions and polynomials. The study highlights how these operators aid in numerical computations, forming the basis for effective approximation techniques in mathematical and engineering problems. At the end, some mcqs and questions are given which will help them to clear these concepts deeply.

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Second Order Linear Ordinary Differential Equation with Constant Coefficient

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Abstract

In this chapter, the existence and uniqueness of the solutions of second order homogeneous linear ordinary differential equations with constant coefficients is discussed. It is also discussed the condition under which the given solutions of second order linear differential equations with constant coefficients are linearly dependent and linearly independent. To explain these concepts, some illustrations are solved.

Key Words: existence and uniqueness of the solutions, constant coefficients, linearly dependent, linearly independent solutions.

1. Introduction

Second order homogeneous linear ordinary differential equations with constant coefficients play very important role in mathematical modelling of many physical phenomena. So, it is very important to study them in details. To find the solution of these types of equations, one needs to find its characteristics equation and find the roots of that characteristic equation. Depending upon the type of roots whether real or complex, we can find the general solution of corresponding Second order homogeneous linear ordinary differential equations with constant coefficients.

2. Preliminaries

In this section, we give some basic definitions.

2.1 Linear differential equation of order n with constant coefficients

A Linear differential equation of order n with constant coefficients is an equation of the form

$$a_0\, y^{(n)} + a_1 y^{(n-1)} + a_2 y^{(n-2)} + \dots\dots + a_n y = b(x)$$

where $a_0 \neq 0$, a_1 , a_2 ,……, a_n are complex constants & b is complex valued function on interval I :a < x <b

2.2 Homogeneous Linear ordinary differential equation of order n with constant coefficients

A Linear differential equation of order n with constant coefficients is an equation of the form

$$a_0\, y^{(n)} + a_1 y^{(n-1)} + a_2 y^{(n-2)} + \dots\dots + a_n y = 0$$

where $a_0 \neq 0$, a_1 , a_2 ,……, a_n are complex constants.

2.3 Non-Homogeneous Linear ordinary differential equation of order n with constant coefficients

A Linear differential equation of order n with constant coefficients is an equation of the form

$$a_0\, y^{(n)} + a_1 y^{(n-1)} + a_2 y^{(n-2)} + \dots\dots + a_n y = b(x)$$

where $a_0 \neq 0$, a_1 , a_2 ,……, a_n are complex constants and b(x) is complex valued function on interval I :a < x <b

2.4 Differential operator of order n with constant coefficients

The operator L is defined by

$L(\emptyset) = \emptyset^{(n)} + a_1\, \emptyset^{(n-1)}(x) + a_2\, \emptyset^{(n-2)} + a_3\, \emptyset^{(n-3)} + \dots\dots + a_n\emptyset$

is called differential operator of order n with constant coefficients. The equation L(y)=b(x) is called non homogenous equation. If b(x)=0 for all X in I corresponding equation L(y)=0 is called homogenous equation.

2.5 Linear Independence

A set of n real or complex functions $f_1, f_2, f_3, \dots, f_n$ defined on an interval (a,b) is said to be linearly independent if when

$c_1 f_1(x) + c_2 f_2(x) + c_3 f_3(x) + \dots\dots + c_n f_n(x) = 0$

for every x in (a,b) implies $c_1 = c_2 = c_3 = \dots = c_n = 0$ Where $c_1, c_2, c_3, \dots, c_n$ are constant.

2.6 Linear Dependence

Given the functions $f_1, f_2, f_3, \dots, f_n$ if constants $c_1, c_2, c_3, \dots, c_n$ not all zero exist such that

$c_1 f_1(x) + c_2 f_2(x) + c_3 f_3(x) + \dots\dots + c_n f_n(x) = 0$ for every x in (a, b), then these functions are linearly dependent.

There are two notions of linearly independence, according as we allow the coefficients c_k $(k = 1,2,3,.....n)$ to assume only real values or also complex values. In the first case, one says that the functions are linearly independent over the field of reals; in the second case, that they are linearly independent over the complex field.

2.7 Wronskian of the n functions:

Assume that each of the functions $f_1(x), f_2(x), f_3(x), \cdots.., f_n(x)$ are differentiable atleast $(n-1)$ times in the interval (a, b). Then the determinant

$$\begin{vmatrix} f_1(x) & f_2(x) & f_3(x) & \cdots & f_n(x) \\ f_1'(x) & f_2'(x) & f_3'(x) & \cdots & f_n'(x) \\ f_1''(x) & f_2''(x) & f_3''(x) & \cdots & f_n''(x) \\ \vdots & \vdots & \vdots & & \vdots \\ f_1^{(n-1)}(x) & f_2^{(n-1)}(x) & f_3^{(n-1)}(x) & \cdots & f_n^{(n-1)}(x) \end{vmatrix}$$

denoted by $\mathrm{W}(f_1, f_2, f_3, \dots, f_n)(x)$ is called the wronskian of the n functions $f_{1,}, f_2, f_3, \dots, f_n$.

3. Main Results

In this section, we have proved some important theorems to show the existence and uniqueness of the solutions to second Order Differential Equations with Constant Coefficients. Wronskian's method is used to test the linear dependence or independence of solutions to given second Order linear ordinary Differential Equations with Constant Coefficients.

Theorem 3.1 : Let a_1 & a_2 be constants & consider the equation

$$L(y) = y'' + a_1 y' + a_2 y = 0$$

1) If r_1 & r_2 are distinct roots of characteristics polynomial

$$P(r) = r^2 + a_1 r + a_2$$

Then the functions $\emptyset_1(x) = e^{r_1 x}$ and $\emptyset_2(x) = e^{r_2 x}$ are solutions of L(y)=0

2) If r_1 is a repeated root of the characteristics polynomial p(r), then the functions

$\emptyset_1(x) = e^{r_1 x}$ and $\emptyset_2(x) = x e^{r_1 x}$ are solutions of L(y)=0

Proof- Let $\emptyset(x) = e^{rx}$ be a solutions of L(y)=0

$$L(e^{rx}) = (e^{rx})'' + a_1(e^{rx})' + a_2 e^{rx}$$
$$= (r^2 + a_1 r + a_2)e^{rx}$$

$= 0$ if and only if $p(r)=r^2+a_1r+a_2=0$

1) If r_1 and r_2 are distinct roots of p(r) then $L(e^{r_1x}) = L(e^{r_2x})=0$ and $\emptyset_1(x)=e^{r_1x}$ and $\emptyset_2(x)=e^{r_2x}$ are solutions of L(y)=0

2) If r_1 is repeated root of p(r) then

$P(r)=(r-r_1)^2$ and $p'(r)=2(r-r_1)$

$L(e^{rx}) =P(r)e^{rx}$ for all r & x

$\frac{\partial}{\partial r}L(e^{rx})=\frac{\partial}{\partial r}[P(r)e^{rx}]$

$\Rightarrow L(xe^{rx})=[P'(r)+xP(r)]e^{rx}$

At $r=r_1$, $P(r_1)=P'(r_1)=0$

i. e $L(xe^{r_1x}) =0$ thus, showing that xe^{r_1x} is a solution of L(y)=0.

Thus, if r_1 is repeated root of the characteristics polynomial P(r), then the functions $\emptyset_1(x)=e^{r_1x}$ and $\emptyset_2(x)=xe^{r_1x}$ are solutions of L(y)=0

Theorem 3.2: If $\emptyset_1$ and $\emptyset_2$ are two solutions of L(y) =0 then $c_1\emptyset 1 + c_2\emptyset_2$ is also solution of L(y)=0 where, c_1 and c_2 are any two constant
Proof- Let $\emptyset_1$ and $\emptyset_2$ be two solutions of L(y)=0

$L(\emptyset_1) =\emptyset_1'' +a_1\emptyset_1' + a_2\emptyset_1 =0$

$L(\emptyset_2) =\emptyset_2'' +a_1\emptyset_2' + a_2\emptyset_2 =0$

Suppose c_1 and c_2 are any two constants then the function Ø defined by $\emptyset =c_1\emptyset 1+ c_2\emptyset_2$ is also solution of L(y)=0

$L(\emptyset)=(c_1\emptyset_1+c_2\emptyset_2)'' + a_1(c_1\emptyset_1+c_2\emptyset_2)'+ a_2(c_1\emptyset_1+c_2\emptyset_2)$

$= c_1(\emptyset_1'' +a_1\emptyset_1' + a_2\emptyset_1) +c_2(\emptyset_2'' +a_1\emptyset_2' + a_2\emptyset_2)$

$=c_1 L(\emptyset_1) +c_2 L(\emptyset_2)$

$=0$

The function Ø which is zero for all x is also a solution called the trivial solution of L(y)=0

Theorem 3.3 [Existence Theorem]

For any real x_0 and constants α,β , there exists a solution $\emptyset$ of initial value problem

$L(y) = y''+a_1y'+a_2y=0, \quad y(x_0)= \alpha, y'(x_0)= \beta \quad -\infty < x < \infty$

Proof – By theorem 1 there exist two solutions $Ø_1$ and $Ø_2$ that satisfy $L(Ø_1)= L(Ø_2)=0$.

From theorem 2, we know that $c_1Ø_1+c_2Ø_2$ is solution of L(y)=0 .We show that there are unique constants c_1, c_2 such that function $Ø = c_1Ø_1+c_2Ø_2$ satisfies $Ø(x_0)= \alpha$ and $Ø'(x_0)= \beta$

$$Ø(x_0)= c_1Ø_1(x_0) +c_2Ø_2(x_0) = \alpha$$

$$Ø'(x_0)= c_1Ø'_1(x_0) +c_2Ø'_2(x_0) = \beta$$

Above system of equations will have a unique solution c_1, c_2 if the determinant

$$\Delta= \begin{vmatrix} Ø1(x_0) & Ø2(x_0) \\ Ø'1(x_0) & Ø'2(x_0) \end{vmatrix}$$

$$= Ø_1(x_0).\ Ø'_2(x_0)- Ø_2(x_0).\ Ø'_1(x_0)\neq 0$$

By theorem 1 $Ø_1(x)=e^{r_1x}$ and $Ø_2(x)=e^{r_2x}$ are solutions of L(y)=0 for $r_1 \neq r_2$

$$\Delta= e^{r_1x_0}r_2e^{r_2x_0}-e^{r_2x_0}r_1e^{r_1x_0}$$

$$=(r_2-r_1)(e^{(r_1+r_2)x_0}) \neq 0$$

By theorem 1 $Ø_1(x)=e^{r_1x}$ and $Ø_2(x)= xe^{r_1x}$ are solutions of L(y)=0 $r_1 = r_2$

And $\Delta= e^{r_1x_0}[e^{r_1x_0}+x_0r_1e^{r_1x_0}] - x_0e^{r_1x_0}r_1e^{r_1x_0}$

$$=e^{2r_1x_0} \neq 0$$

Thus, the determinant condition is satisfied in both the cases. Therefore, c_1, c_2 are uniquely determined.

The function $Ø = c_1Ø_1+c_2Ø_2$ is desired solution of initial value problem.

The function Ø which is zero for all x is also a solution called the trivial solution of L(y)=0

Theorem 3.3 [Existence Theorem]

For any real x_0 and constants α,β, there exists a solution $Ø$ of initial value problem

$$L(y) = y''+a_1y'+a_2y=0, \quad y(x_0)= \alpha,\ y'(x_0)= \beta \quad -\infty < x < \infty$$

Proof – By theorem 1 there exist two solutions $Ø_1$ and $Ø_2$ that satisfy $L(Ø_1)= L(Ø_2)=0$.

From theorem 2, we know that $c_1Ø_1+c_2Ø_2$ is solution of L(y)=0 .We show that there are unique constants c_1, c_2 such that function $Ø = c_1Ø_1+c_2Ø_2$ satisfies $Ø(x_0)= \alpha$ and $Ø'(x_0)= \beta$

$$Ø(x_0)= c_1Ø_1(x_0)+c_2Ø_2(x_0)=\alpha$$

$$Ø'(x_0)= c_1Ø'_1(x_0)+c_2Ø'_2(x_0)=\beta$$

Above system of equations will have a unique solution c_1, c_2 if the determinant

$$\Delta=\begin{vmatrix}Ø1(x_0) & Ø2(x_0)\\ Ø'1(x_0) & Ø'2(x_0)\end{vmatrix}$$

$$= Ø_1(x_0).\ Ø'_2(x_0)- Ø_2(x_0)\ .Ø'_1(x_0)\neq 0$$

By theorem 1 $Ø_1(x)=e^{r_1x}$ and $Ø_2(x)=e^{r_2x}$ are solutions of L(y)=0 for $r_1 \neq r_2$

$$\Delta= e^{r_1x_0}r_2e^{r_2x_0}-e^{r_2x_0}r_1e^{r_1x_0}$$

$$=(r_2-r_1)(e^{(r_1+r_2)x_0})\neq 0$$

By theorem 1 $Ø_1(x)=e^{r_1x}$ and $Ø_2(x)=xe^{r_1x}$ are solutions of L(y)=0 $r_1=r_2$

And $\Delta= e^{r_1x_0}[e^{r_1x_0}+x_0r_1e^{r_1x_0}]-x_0e^{r_1x_0}r_1e^{r_1x_0}$

$$=e^{2r_1x_0}\neq 0$$

Thus, the determinant condition is satisfied in both the cases. Therefore, c_1, c_2 are uniquely determined.

The function $Ø = c_1Ø_1+c_2Ø_2$ is desired solution of initial value problem.

Theorem 3.5 (Uniqueness Theorem)

Letα,β be any two constants and let x_0 be any real number. On any interval I containing x_0 there exist at most one solution Ø of initial value problem

$$L(y) = y''+a_1y'+a_2y=0, \quad y(x_0)=\alpha,\ y'(x_0)=\beta \quad -\infty < x < \infty$$

Proof – Suppose $\emptyset$ and ψ are two solutions.

Let $\theta = \emptyset - \psi$.

Since $L(\theta) = L(\emptyset) = L(\psi)=0$

$$L(\theta) = L(\emptyset - \psi)= L(\emptyset) - L(\psi)=0$$

Since $\emptyset(x_0) = \psi(x_0)= \alpha$ and $\emptyset'(x_0) = \psi'(x_0)= \beta$

$$\theta(x_0) = \emptyset(x_0) - \psi(x_0)= 0$$

And $\theta'(x_0)= \emptyset'(x_0) - \psi'(x_0)=0$

$$L(\theta) = 0, \quad \theta(x_0)=0, \text{ and } \theta'(x_0)=0$$

$$\|\theta(x_0)\|^2 =[|\theta(x_0)|^2 + |\theta'(x_0)|^2]=0$$

By initial value theorem, we see that

$\|\theta(x)\|$ =[| $\theta(x_0)|^2$ + $|\theta'(x_0)|^2$]=0 for all x in I

This implies $\theta(x)$ = 0 for all x in I.

Lemma 3.6: A set of real valued functions on an interval (a, b) is linearly independent over the complex field if and only if it is linearly independent over the real field.

Proof: If the set of real valued functions on an interval (a, b) is linearly independent over the complex field, then it is linearly independent over the field of reals.

Conversely suppose the set is linearly independent over the real field. Therefore for $\alpha_j \in R, \sum_{j=1}^{n} \alpha_j f_j(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x) + \alpha_3 f_3(x) + \cdots + \alpha_n f_n(x) = 0$ for all x in (a, b) implies $a_j = 0$ for all $j = 1,2,3$ ..., n . Let $\sum_{j=1}^{\pi} c_j f_j(x) = 0$ for all x in (a, b) and for some $c_j \in C. j = 1,2,3 \cdots, n$. Since the function f_j are real valued and $\Sigma c_j f_j(x) = 0$.

$$[\Sigma c_j f_j(x)]^* = 0. \text{ implies } \sum_{j=1}^{n} c_j{}^* f_j(x) = 0. \text{ Thus, } \sum_{j=1}^{n} \left(\frac{c_j - c_j{}^*}{i}\right) f_j(x) = 0. \text{ But } (c_j - c_j{}^*)/i$$

are all real and the set is linearly independent over the real field therefore $c_j = c_j{}^*$. But then $c_j{}'$ s Differential Equat ions are all real therefore $\sum_{j=1}^{n} c_j f_j(x) = 0$ implies $c_j = 0$ for $j = 1,2, \ldots . n$. A set of functions which is linearly dependent on a given dounain may become linearly independent when the functions are extended to a larger domain. However, a linearly independent set of functions clearly remain linearly independent on the restricted domain.

Theorem 3.7 Let a_1, a_2 be constants and consider the equation $L(y) = y'' + a_1 y' + a_2 y = 0$. The two solutions of $L(y) = 0$ given in the theorem 1.1.1 are linearly independent on any interval I.

Proof : Let r_1, r_2 be the roots of characteristic polynomial $p(r) = r^2 + a_1 r + a_2$.

Case 1.

If $r_1 \neq r_2$, then $\phi_1(x) = e^{r_1 x}$ and $\phi_2(x) = e^{r_2 x}$ are two solutions of the equation $L(y) = 0$ on an interval I.
Suppose $c_1 e^{r_1, x} + c_2 e^{r_2 x} = 0$ for all x in I .
Then $c_1 + c_2 e^{(r_2 - r_1)x} = 0$ for all x in I.
Differentiation of above equation with respect to x gives $c_2(r_2 - r_1)e^{(r_2 - r_1)x} = 0$ for all x in I.
Since, $r_2 \neq r_1$ and exponential function in non-zero, c_2 is zero. But if c_2 is zero then $c_1 + c_2 e^{(r_2 - r_1)x} = 0$ implies c_1 is zero. Thus, $c_1 e^{r_1 x} + c_2 e^{r_2 x} = 0$ implies $c_1 = c_2 = 0$.
Therefore $\phi_1(x) = e^{r_1 x}$ and $\phi_2(x) = e^{r_2 x}$ are linearly independent.
Case 2.
If $r_1 = r_2$, then $\phi_1(x) = e^{r_1 x}$ and $\phi_2(x) = x e^{r_1 x}$ are two solutions of the equation $L(y) = 0$ on an interval I.
Suppose $c_1 e^{e_1 x} + c_2 x e^{r_2 x} = 0$ then $c_1 + c_2 x = 0$ for all x in I. Therefore $c_1 = c_2 = 0$. Thus, ϕ_1 and ϕ_2 are linearly independent
Thus, in both cases the two solutions ϕ_1 and ϕ_2 of $L(y) = 0$ are linearly independent.

Theorem 3.8 : Two solutions ϕ_1, ϕ_2 of $L(y) = 0$ are linearly independent on an interval I if and only if $\mathrm{W}(\phi_1, \phi_2)(x) \neq 0$ for all x in I .
Proof: Suppose $\mathrm{W}(\phi_1, \phi_2)(\mathrm{x}) \neq 0$ for all x in I
Let c_1, c_2 be constants such that

$$c_1\phi_1(x) + c_2\phi_2(x) = 0 \text{ for all } x \text{ in I. Then}$$
$$c_1\phi_1'(x) + c_2\phi_2'(x) = 0 \text{ for all } x \text{ in I.}$$

Above two equations can be written as

$$\begin{bmatrix} \phi_1(x) & \phi_2(x) \\ \phi_1'(x) & \phi_2'(x) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Since, $\mathrm{W}(\phi_1, \phi_2)(x) \neq 0$ for all x in I, the coefficient matrix is invertible. On premultiplying the inverse of the coefficient matrix results in $c_1 = c_2 = 0$. This proves that ϕ_1 and ϕ_2 are linearly independent on I.
Conversely, assume that ϕ_1, ϕ_2 are linearly independent on I. Suppose that there is a point x_0 in I such that $\mathrm{W}(\phi_1, \phi_1)(x_0) = 0$. Then the system of equations

$$\begin{bmatrix} \phi_1(x_0) & \phi_2(x_0) \\ \phi_1'(x_0) & \phi_2'(x_0) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

has a solution c_1, c_2 where at least one of these numbers is not zero. Let c_1, c_2, be such a solution and consider the function $\psi(x) = c_1\phi_1(x) + c_2\phi_2(x)$. Now

$L(\psi) = 0$ and $\psi(x_0) = 0, \psi'(x_0) = 0$. Therefore $\|\psi(x_0)\| = [|\psi(x_0)|^2 + |\psi'(x_0)|^2]^{\frac{1}{2}} = 0$. By theorem 1.1.4 $\|\psi(x)\| = 0$. But $\|\psi(x)\| = [|\psi(x)|^2 + |\psi'(x)|^2] = 0$. Therefore $\psi(x) = 0$ for all x in I and thus $c_1\phi_1(x) + c_2\phi_2(x) = 0$ for all x in I. But then ϕ_1 and ϕ_2 are linearly dependent. Thus, the supposition $\mathrm{W}(\phi_1, \phi_2)(x_0) = 0$ must be false and therefore $\mathrm{W}(\phi_1, \phi_2)(x) \neq 0$ for all x in I .

In the next theorem we will prove that we need to compute $\mathrm{W}(\phi_1, \phi_2)$ at only one point to test the linear independence of the solutions ϕ_1 and ϕ_2.

Theorem 3.9: Let ϕ_1, ϕ_2 be two solutions of $L(y) = 0$ on an interval I and let x_0 be any point in I. Then two solutions ϕ_1 and ϕ_2 are linearly independent on I if and only if $\mathrm{W}(\phi_1, \phi_2)(x_0) \neq 0$.

Proof: If ϕ_1 and ϕ_2 are linearly independent on I then by theorem 1.2.2, $\mathrm{W}(\phi_1, \phi_2)(x) \neq 0$ for all x in I. In particular $\mathrm{W}(\phi_1, \phi_2)(x_0) \neq 0$ conversely, suppose $\mathrm{W}(\phi_1, \phi_2)(x_0) \neq 0$ and suppose c_1, c_2 are constants such that $c_1\phi_1(x) + c_2\phi_2(x) = 0$ for all x in I. Then $c_1\phi_1(x_0) + c_2\phi_2(x_0) = 0$ and $c_1\phi_1'(x_0) + c_2\phi_2'(x_0) = 0$.

i.e.

$$\begin{bmatrix} \phi_1(x_0) & \phi_2(x_0) \\ \phi_1'(x_0) & \phi_2'(x_0) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

But since the determinant of the coefficient is $\mathrm{W}(\phi_1, \phi_2)(x_0) \neq 0$ we obtain $c_1 = c_2 = 0$.

Thus ϕ_1, ϕ_2 are linearly independent on I.

In the next theorem we show that the knowledge of two linearly independent solutions of $L(y) = 0$ is sufficient to generate all solutions of $L(y) = 0$.

Theorem 3.10:

Let ϕ_1, ϕ_2 be any two linearly independent solutions of $L(y) = 0$ on an interval I. Every solution ϕ of $L(y) = 0$ can be written uniquely as

$\phi = c_1\phi_1 + c_2\phi_2$ where c_1, c_2 are constants.

Proof : Let x_0 be a point in I. Let $\phi(x_0) = \alpha, \phi'(x_0) = \beta$. Since ϕ_1, ϕ_2 are linearly independent on I we know that $\mathrm{W}(\phi_1, \phi_2)(x_0) \neq 0$. Consider the two equations.

$$\begin{bmatrix} \phi_1(x_0) & \phi_2(x_0) \\ \phi_1'(x_0) & \phi_2'(x_0) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Since $\mathrm{W}(\phi_1, \phi_2)(x_0) \neq 0$, above system of equations has a unique solution c_1, c_2. For this choice of c_1, c_2 the function $\psi(x) = c_1\phi_1(x) + c_2\phi_2(x)$ satisfies

$\psi(x_0) = c_1\phi_1(x_0) + c_2\phi_2(x_0) = \alpha = \phi(x_0)$ i.e. $\psi(x_0) = \phi(x_0)$ similarly $\psi'(x_0) = \phi'(x_0)$ and $L(\psi) = 0$. From the uniqueness theorem 1.1.5 it follows that $\psi = \phi$ on I i.e. $\phi = c_1\phi_1 + c_1\phi_2$.

4. Illustrations

1) Find all solutions of the following equations y'- 4y=0

⇒ The characteristics polynomial is p(r) = r^2-4.

r_1=2 and r_2 = -2 are two distinct roots of P(r)=0.

Ø$_1$(x)=e^{2x} and Ø$_2$(x)=e^{-2x} are solutions of L(y)=0.

For any constants c_1 and c_2 , c_1e^{2x} + c_2e^{-2x} is a solution.
Thus the general solution is Ø(x)= c_1e^{2x} + c_2e^{-2x}

2) y''+2ir+1 =0

⇒ The characteristics polynomial p(r)= r^2+2ir+1

P(r)=0 ⇒r=$\frac{-b\pm\sqrt{b^2-4ac}}{2a}$

⇒r= $\frac{-2i\pm\sqrt{2i^2-4(1)(1)}}{2(1)}$

⇒ r=$\frac{-2i\pm\sqrt{-8}}{2}$

⇒r= (-1±$\sqrt{2}$)i

Thus r_1 = (1+$\sqrt{2}$)i and r_2 = (1-$\sqrt{2}$)i
Are two distinct roots of p(r)=0
Therefore Ø$_1$(x)= $e^{(-1+\sqrt{2})ix}$ and Ø$_2$(x)=$e^{(-1-\sqrt{2})ix}$ are two solutions.
Thus, for any constants c_1 and c_2 ,
Ø(x)= $c_1e^{(-1+\sqrt{2})ix}$ + $c_2e^{(-1-\sqrt{2})ix}$ is a general solution.

3) y'' -2y'+4y=0
⇒ The characteristics polynomial is p(r)= r^2 -2r + 4
P(r) = $(r-2)^2$
⇒ r_1 = 2 and r_2 =2 are repeated roots of P(r) =0
Therefore Ø$_1$(x) = e^{2x} and Ø$_2$(x) = xe^{2x} are solutions of L(y)=0
Thus, for any constants c_1 and c_2 ,
Ø(x)= c_1e^{2x} + c_2 xe^{2x} is general solution of L(y)=0

4) Find the solutions Ø of the following initial value problems

Ø'' + Ø' -6Ø=0 ,Ø(0)= 1 & Ø'(0)= 0

⇒ The characteristics polynomial P(r) = r^2 + r- 6.

r_1 =2 and r_2= -3 are distinct roots

Ø(x)= $c_1 e^{2x}$ + $c_2 e^{-3x}$ is general solutions

Ø (0)= 1 ⇒ c_1+c_2 =1 …………(1)

Ø'(0)= 0 ⇒ Ø'(x) =2c_1 e^{2x} -3$c_2 e^{-3x}$ at x=0

⇒ Ø'(0) = 2c_1 – 3c_2 = 0 ………(2)

Solving equation (1) & (2) for c_1 and c_2 we get $c_1 = \frac{3}{5}$ and $c_2 = \frac{2}{5}$

Thus, the required solution is Ø(x)= $\frac{3}{5} e^{2x} + \frac{2}{5} e^{-3x}$

5) Show that the functions e^x, e^{2x}, e^{3x} are linearly independent.

Ans. : Method 1:

Let $c_1 e^x + c_2 e^{2x} + c_3 e^{3x} = 0$

then $c_1 + c_2 e^x + c_3 e^{2x} = 0$

Differentiate above equation (1) with respect to x then $c_2 e^x + 2c_3 e^{2x} = 0$ implies

$$c_2 + 2c_3 e^x = 0$$

By differentiating equation (2) with respect to x we get $2c_3 e^x = 0$ therefore $c_3 = 0.$

But then by equation (2) $c_2 = 0$ and by equation (1) we get $c_1 = 0$. Thus $c_1 = c_2 = c_3 = 0.$

Therefore the functions e^x, e^{2x}, e^{3x} are linearly independent.

Method 2:

Let

$$\phi_1(x) = e^x, \phi_2(x) = e^{2x}, \phi_3(x) = e^{3x}$$

$$\mathrm{W}(\phi_1, \phi_2, \phi_3) = \begin{vmatrix} e^x & e^{2x} & e^{3x} \\ e^x & 2e^{2x} & 3e^{3x} \\ e^x & 4e^{2x} & 9e^{3x} \end{vmatrix} = e^x e^{2x} e^{3x} \begin{vmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \\ 1 & 4 & 9 \end{vmatrix}$$

$$= e^{6x}[1(18-12) - 1(9-3) + 1(4-2)]$$

$$= 2e^{6x} \neq 0.$$

By theorem 1.2.2 ϕ_1, ϕ_2, ϕ_3 are linearly independent.

5. Conclusion

In this chapter, author had tried to give proofs of important theorems related to the existence and uniqueness of the solution to general second order homogeneous linear ordinary differential equations with constant coefficients. Wronskian's method is used to determine whether given two solutions of second order homogeneous ODE with constant coefficients are linearly dependent or independent. Some illustrations are given by using the theorems proved in this chapter.

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