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Biomedical Intelligence Overview

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Abstract

The fourth industrial revolution is advancing, and biomedical intelligence is developing quickly to fill the gap between engineering and many biological and medical disciplines. With its use in diagnostics, drug development, genomics, predictive analysis, personalised medicine, robotic surgery, upgrading POC and IoMT devices, and its significant advancement in contemporary healthcare systems, BI is expanding its market.

In this chapter's overview, we will primarily discuss BI history, perspective, application, future potential, and challenges related to it, such as data security, inter predictability, transparency, etc., with the goal of achieving effective patient diagnosis through early disease prediction.

We will go further into the artificial intelligence (AI) techniques that can examine various medical diseases, such as machine learning, artificial neural networks, deep learning, and fuzzy logic systems.

Keywords: Biomedical Intelligence, Diagnostics, Drug Discovery, Modern Healthcare Systems, Machine Learning, Artificial Neural Networks, Deep Learning, Fuzzy Logic system.

Introduction

Overview of AI History

Historical perspective of AI arises back in 1920 when robot word was introduced. The term AI was coined by John Mac Carthy in 1956 when he developed LISP programme language for AI in 1958 and from then till present era AI saw advancements in various disciplines. In 2006, Geoffrey and his colleagues developed methodology for addressing gradient vanishing problems thus building of neural network leading to deep learning and machine learning algorithms that enabled computer system to become intelligent.

There are three broad classification of AI on basis of it's functionalities and capabilities namely Artificial super intelligence (ASI), AGI (Artificial General intelligence or strong AI) and ANI (Artificial Narrow intelligence or weak AI).

ANI as it's name suggest it functions only to in specific domain like recognizing image of tumors or fractures in X-rays, MRIs, or CT scans but can't perform tasks outside of this domain. Siri, chatboats, voice chatting etc are some other examples.

AGI mimics human intellect and have consciousness to generalized it's learning in different areas like machines that learn to analyze and extract useful patterns from large data volumes and automation technologies and both of these AI's different AI devices are designed based on different algorithms.

ASI represents the pinnacle of AI development as it's intelligence surpasses human intelligence with it's ability to mimic human brain and outhink it.

The development of artificial intelligence (AI) has changed the world, particularly in the last ten years. It has becoming easier to incorporate AI into particular areas as a result of the increase in processing capacity and the democratization of AI tools. The medical industry is proof of these developments.

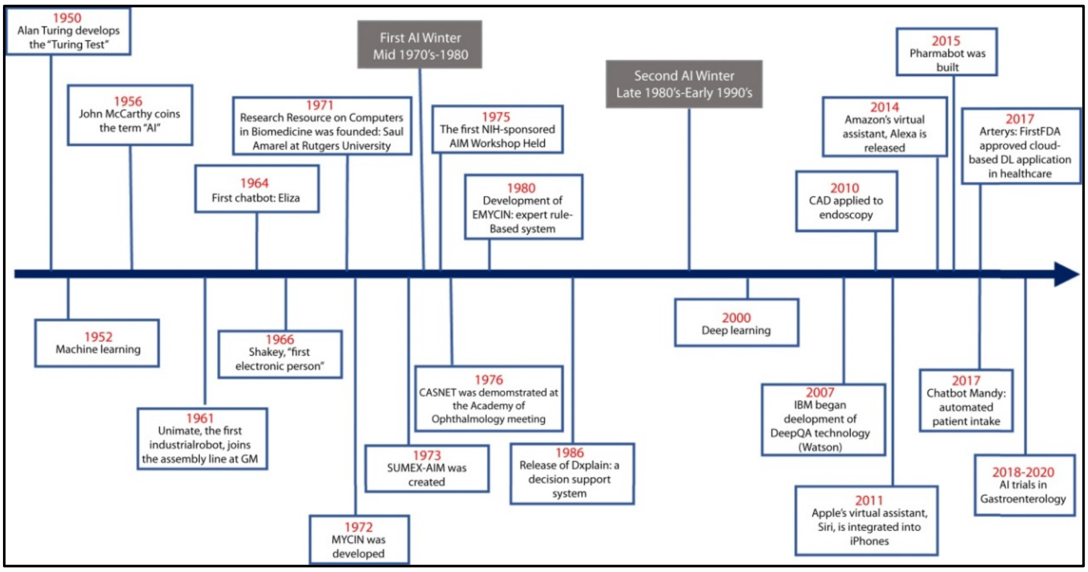

Figure 1: History of AI in Healthcare

1. Foundations of AI in Biomedical Intelligence

During the 1960s and 1970s with the deployment of groundbreaking expert systems like Dendral and MYCIN AI was first used in field of biomedical sciences which led to the evolution of term biomedical intelligence. Then in 2000 with completion of first human genome project (HGP) the explosion occurs in omics digital data namely genomics, proteomics and metabolomics which lead to the development of cancer studies, personalized medicine therapy, drug discovery and the list goes on.

As every AI DEVICES have different application in medical science due to different healthcare data like clinical data, medical imaging data, omics data (genomics, proteomics and metabolomics) they work on different algorithms based on Deep learning ,Machine learning, and Fuzzy logic approach to predict, interpret, analyze and produced data with great interpretability, transparency, security and accuracy.

1.1 Modern Healthcare

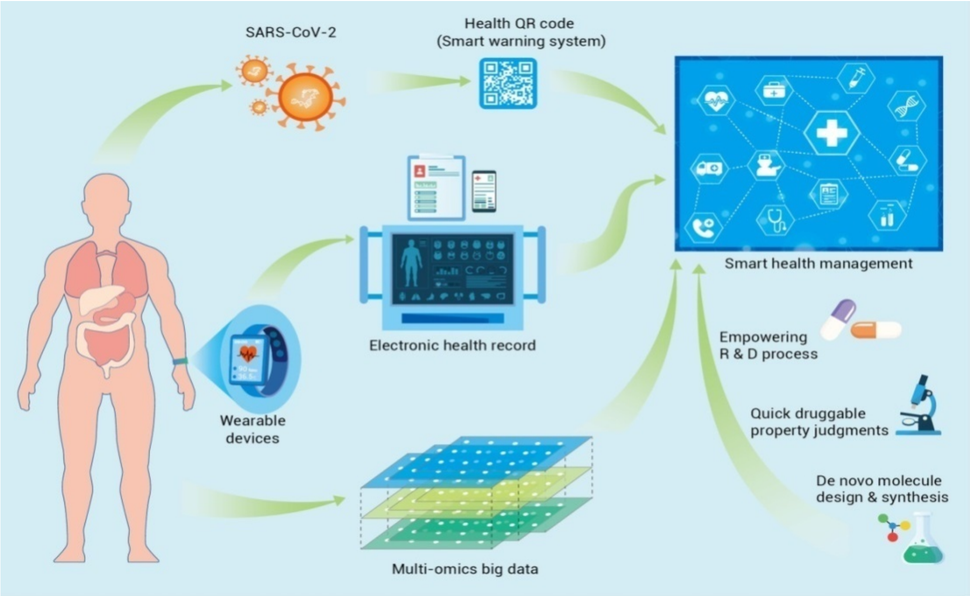

Figure 2: Modern Healthcare Management System

1.2 Revolutionizing Healthcare with AI Insights

AI-driven data analysis is revolutionizing healthcare across multiple fronts. Machine learning and deep learning algorithms process vast clinical datasets, including electronic health records (EHRs) which arise due to explosion of Genomics data, Medical Imaging , clinical diagnostics, specific biomarkers or signaling molecule from disease condition are the reason of progression of modern healthcare which emphasizes a comprehensive, patient-centered approach to predict clinical outcomes, ranging from treatment benefits to post-surgical risks. These insights empower hospitals by optimizing resource allocation, reducing wait times, and enhancing healthcare quality. Furthermore, AI monitors real-time patient data from various settings, quickly detecting anomalies and predicting critical events like cardiac arrest. This timely intervention significantly improves patient care and safety.

1.3 Advancing Personal Health with Wearable Biosensors

Wearable biosensors, including implantable devices and wearables like smartwatches, provide continuous monitoring of vital health parameters and enable early disease detection. From tracking glucose levels with implantable sensors to assessing sleep quality and heart rhythms with wearable gadgets, these technologies empower individuals to manage their health conveniently. This trend is poised for further growth, with biosensors being integrated into a wide range of accessories, promising even more accessible and comprehensive health monitoring.

1.4 Applications in Various Medical Fields

AI has expanded its applications to various medical fields beyond radiology and histopathology. It can accurately characterize cardiomyopathies through electrocardiograms, identify skin lesions through dermatological images, diagnose eye conditions through ophthalmological images, and detect colon polyps through endoscopy images.

1.5 AI in Surgical Robotics

Surgical robotics is an area of rapid development in AI. Surgical robotic systems have been introduced in operating rooms, assisting surgeons during procedures. For example, the da Vinci® Surgical System offers precision in surgical motions and the elimination of tremors. Autonomous robots capable of performing specific tasks in surgery are also being developed, potentially automating various medical procedures in the future.

1.6 AI in Biomedical Imaging

DL algorithms, including (ANNs) Artificial Neural Networks comprising multiple hidden layers, are competent of rapidly and accurately analyzing medical scans. Radiology has been a major beneficiary of AI, with DL algorithms being used to interpret various types of Medical images, such as X-rays, CT scans, mammograms, and MRI images. It can accurately characterize cardiomyopathies through electrocardiograms, identify skin lesions through dermatological images, diagnose eye conditions through ophthalmological images, and detect colon polyps through endoscopy images. These algorithms can detect a wide range of pathological conditions, including lung diseases, Fractures, Cerebral hemorrhages, Breast cancer etc.

1.7 Point of Care device(POC)) &Internet of Medical Things(IoMT)

The advanced medical understanding led to advancement of modern healthcare system like of the personalized medicine, drug discovery, Robotic surgery, Wearable health devices like (IoMT and POC), Telemedicine, Virtual Heath assistance, Predictive analysis, Natural Language processing etc whichpresent the future outlook in modern healthcare.

The synergy of AI with the Internet of Medical Things (IoMT), complemented by Point-of-Care (POC) devices, is heralding a new era in healthcare. This integration not only elevates the precision, functionality, and risk evaluation of contemporary medical tools but also lays the foundation for the next wave of biomedical systems. These systems are designed with a keen emphasis on timely medical interventions and outcomes that resonate with individual patient needs.

Moreover, the fusion of POC devices into portable diagnostic instruments is a game-changer. It offers the luxury of instant, location-flexible medical testing, diminishing the traditional reliance on centralized laboratories. This accelerates the diagnostic process, ensuring prompt treatments. In summation, with AI at the helm, healthcare is evolving into a domain that's more immediate, efficient, and tailored to individual needs

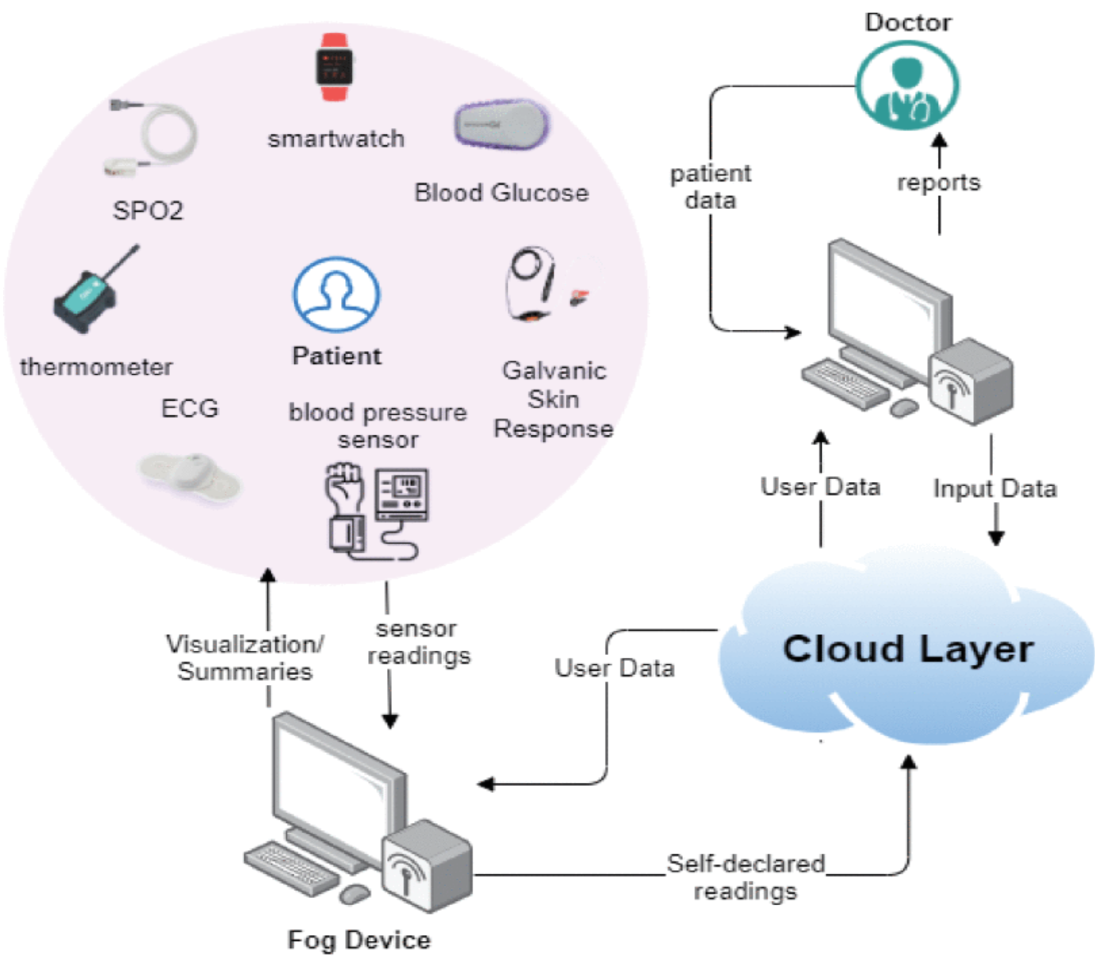

Figure 3: General Framework of IoMT devices

1.8 Telemedicine

The development of telemedicine has increased access to healthcare, and the field's continued development emphasizes the significance of continuing study and adaptation. Modern healthcare, in the context of biomedical intelligence, not only makes use of technology and research to improve patient care, but also acknowledges the global character of health concerns and promotes international partnerships and efforts. In essence, biomedical intelligence's depiction of contemporary healthcare is a dynamic interaction between technology, research, and patient-centered care.

2. AI Algorithms Used in Different Domain of Healthcare System

Data disease, diagnosis and digital therapeutics have always been abundant in the medical industry, from patient records to sophisticated imaging. It was difficult to process, examine, and draw significant conclusions from this data, though. This divide has been filled in by subsequent improvements in computers. Large and complicated medical information may now be mined for patterns and insights thanks to high-performance computing and sophisticated algorithms.

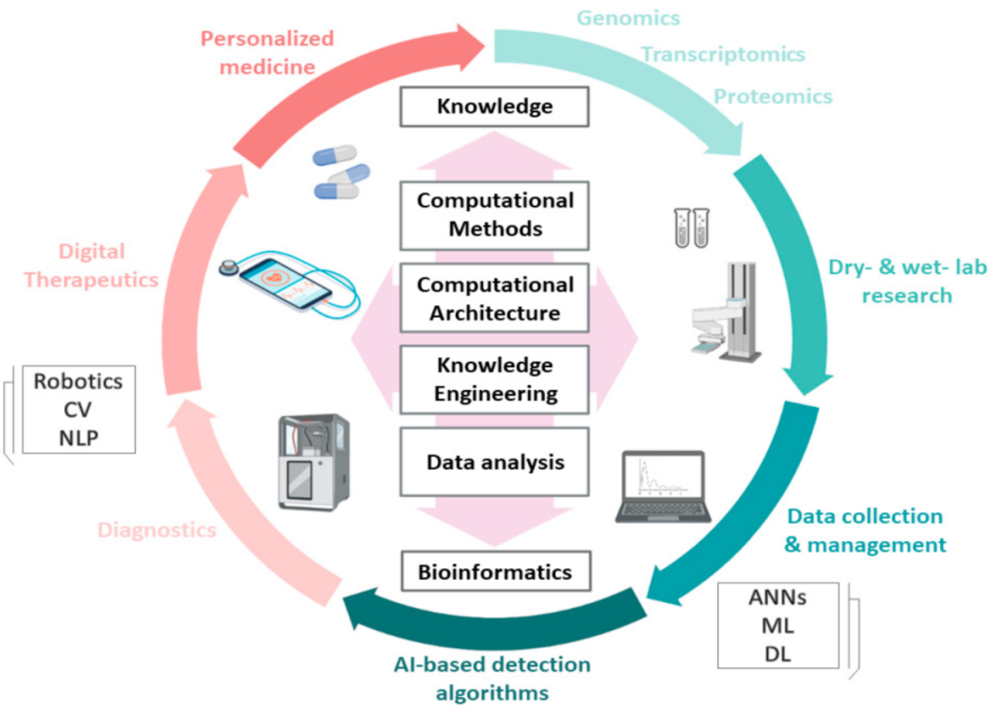

Figure 4: AI tools used in different disciplines of Biomedical sciences

Advanced algorithms, encompassing Machine Learning, Artificial Neural Networks, and Fuzzy Logic, are redefining conventional healthcare practices, ushering in a more patient-focused approach.

Different algorithm based AI devices are streamlining complex and laborious tasks and is reducing the need for manual human oversight in areas of healthcare that traditionally dependent on human intellect.

We will now understand the different AI algorithms based on certain anologies of day to day life and then dwell deep inside each of them. We will discuss the algorithms which are majorly used in medical applications:-

2.1 Machine Learning

The Concept of machine learning algorithm lies in utilizing training for making decision or prediction from the large volume data without being specifically programmed for that particular task.

Analogy: Let's suppose we're teaching a child to differentiate between cat and dog by showing them only their pictures. Thus when they witness the same, the child could easily tell that is a cat or a dog without being seeing them before in real. The training in machine learning model is analogus to above example.

Machine Learning has three approaches namely Supervised , Unsupervised and Reinforcement Learning. These models fetch upon different datasets to build models, classify data and to achieve maximum output . Each of these subset is defined below:-

2.1.1 Supervised Machine Learning (SML)

In SML the algorithms are trained using labeled data . The model uses the labels associated with each input data in learning the associated pattern. When the model makes mistakes in recognizing the patterns than backpropogation act as feedback system which figures out some parameters on which the machine needs to work or adjust so as to produce better output. Backpropogation is an algorithm which automates this feedback and adjustment process. Once the training get's complete on labeled data the model then looks at new unlabeled datasets for predictive modelling.

It include methods like Support Vector Learning (SVM), Decision Tress, Relevant vector machines (RVM) and Random Forest.

- **Challenges**

The shortcomings of ML arises as overfitting due to modelling error when the model starts mistaking irrelevant data as underlying patterns because of memorising irrelevant data rather than understanding it as irrelevant. It happens when When ML is trained on particular dataset too closely that it starts recognising noise and random fluctuation as a part of it . Eventually it struggles to generalize new unseen data and performs poorly.

- **Solutions to overfitting**

Solution	Description
Cross-validation:	It involves splitting of data into multiple sets instead of splitting into one set and validating the model performance against each split.
Data Augmentation:	By making certain modification indata we can increase the amount of existing data. For images, this might mean rotating, zooming, or flipping the image.
Regularization	It reduces the overcomplexity by adding penalty each time the logarithm goes wrong thus discouraging overfitting.
Ensemble Modelling	Combining multimodal approach and their predictions to reduce the potential biasness in final output.

Applications Supervised Machine Learning

- **Categorization:** Classification Algorithms categorize input data into predefined classes. e.g. detection of clinical diseases. Classifications can be binary (e.g., disease/healthy), ternary, or quaternary (e.g., different tumor grades).
- **Predictive Modeling:** Regression Algorithms predict numerical outcomes based on input data e.g. Predictive models in healthcare for disease prediction and drug discovery.

2.1.2 Unsupervised Machine learning

In USML model, bunch of data is fetched without labeling(unlabeled data) to make it finds patterns or classify the data on it’s ownby clustering approach.

The unlabeling feature of data help to reduce cost , time, analyze continuous incoming data and help to do exploratory analysis of data when we aren't sure of any patterns that might exist in our data. Thus USML model is more suistainable as compared to other ML approaches.

The table given below highlights type of USML techniques along with their description

Technique	Type	Description
K-Clusturing	Clustering of common data points.	It involves grouping of data on the basis of some common parameters and partition data into 'K' clusters where each data point belongs to the cluster with the closest mean.
Gaussian's mixture models	Clustering of common data points.	It sorts data into groups but also acknowledge the ambiguity in data and assumes data to be mixture generated from a of several Gaussian distributions.
Principle Component Analysis.	Dimensionality Reduction	Not strictly a clustering method. It reduce the number of variables or features in the dataset while preserving as much information as possible by looking for most standout feature in mixture of data. PCA analyze the principle component and maximize it's variance . By continuing in this way it simplifies the data by reducing it's dimensions thus maximizing information.

- **Challenge**

As there's no guidance or right answer provided to the model unlike SML, USML might produce non- intuitive grouping of data.

- **Applications of Unsupervised Machine Learning**

1. Medical Image Detection: Grouping similar images, like identifying types of tumors from MRI scans without pre-defined categories.
2. Anomaly Detection: Identifying rare events, like a sudden outbreak of a disease.
3. Drug Discovery: Finding patterns in how different compounds react without having prior categories.
4. Genomics: Grouping genes or proteins based on their functions or structures without pre-defined categories.

2.1.3 Reinforcement Learning

The computer learns by trial and error through interacting with its environment, aiming to achieve the maximum reward thus every task it learns it get's stronger in it's performance. Reinforced learning is a reward/penalty-based learning method. Algorithms assign positive values to desired results and negative values to undesired effects. These algorithms are hard to train and time-consuming.

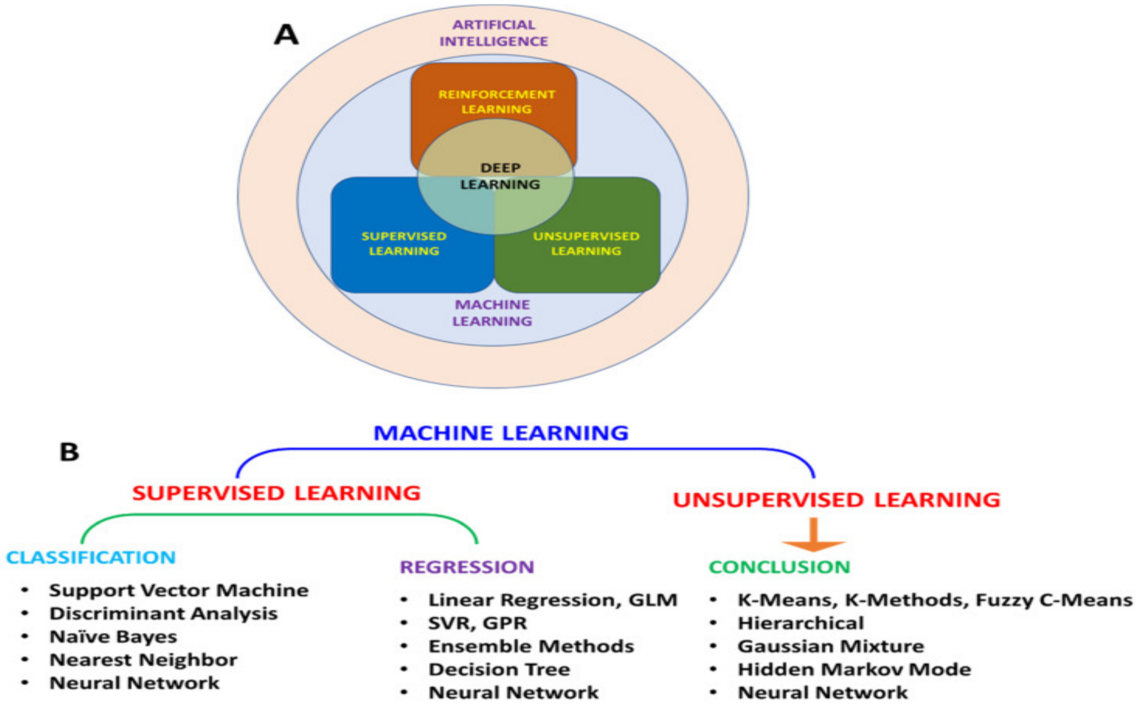

Figure 5: A) Venn diagram representing relation between AI,ML &DL. B) Different approaches of ML

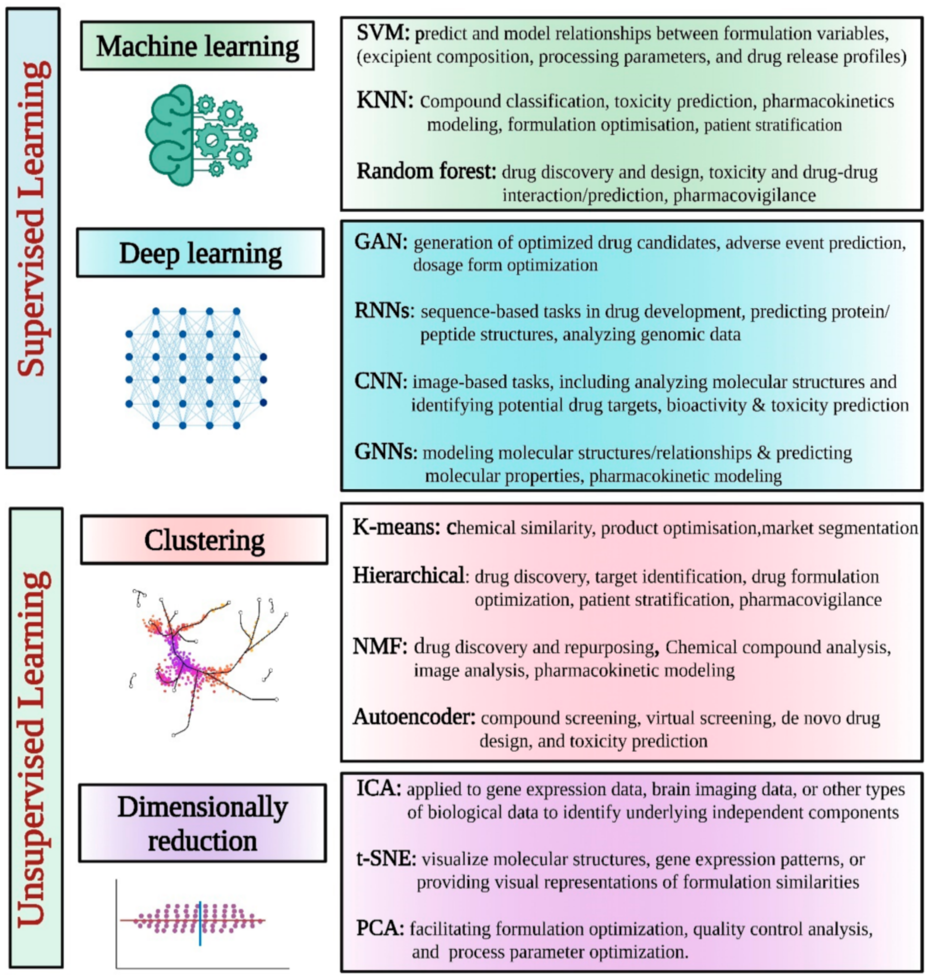

Figure 6: Different Levels of Learning along with their sublevels.

2.2 Deep Learning(DL)

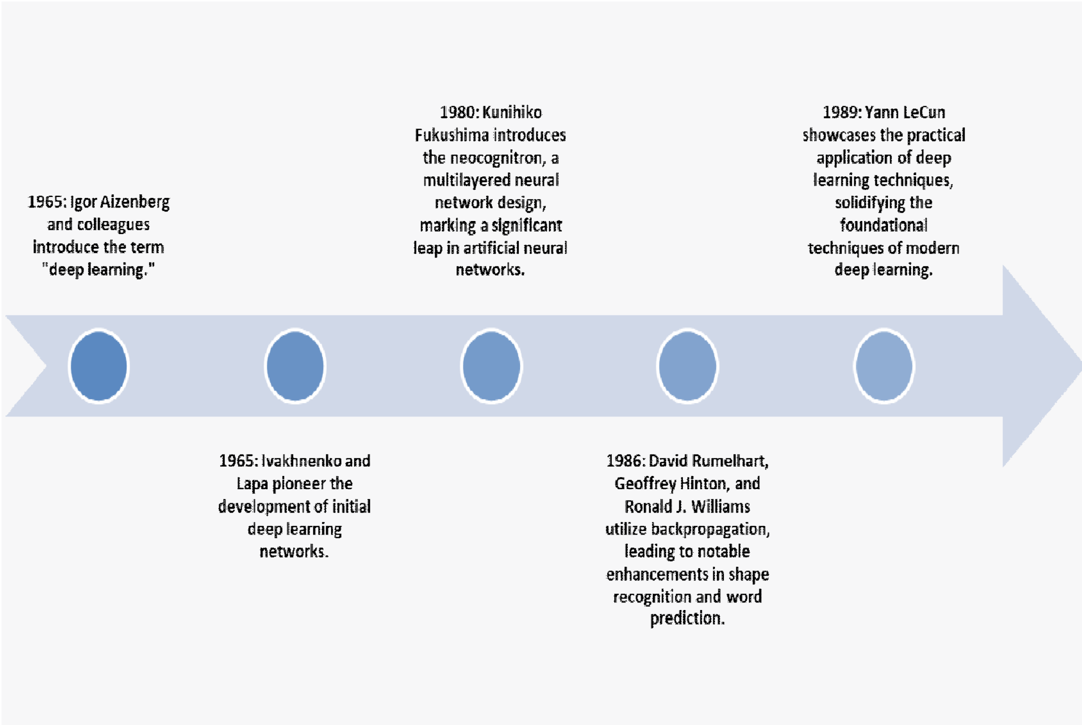

Figure 7: Timeline of Deep Learning evolution.

A more closer approach of ML is Deep Learning as it is a subordinate of machine learning DL mimics human brain in it's functionality. As the interconnection between neurons make the complex processing easy, the same way deep learning algorithm functions to handle super complicated task thus Deep Learning is like building such a multi-roomed, multi-worker factory for computers. This massive amount of data fuels up DL making the algorithm more powerful and accurate. DL uses multiple layers of algorithms in neural networks, mimicking the human brain to analyze patterns by recognizing images. For that, let us understand what does a neural network means.

2.2.1 Artificial Neural Network

McCulloch and Pitts conceptulaised the term ANN .As the name suggest are artificial human neurons forming an input layer, an output layer and in between it forms deep and more hidden layers to process data in order to ensure deep learning alike human brains hence ANN are also known as deep networks. The perceptron was the simplest form of ANN that was attempted by Rosenblatt but it was having feedback/ backpropogation issues which was addressed by Rumelhart that enabled processing of more complex data and draw patterns without manual intervention.

The main architecture of ANN is described in the table below:-

Network Type	Description	Characteristics & Uses	Unique Features	Challenges & Solutions
Convolutional Neural Networks (CNNs)	Networks designed mainly for spatial datasets.	Used for image and spatial data recognition. Contains filters within layers to transform data	Composed of an input layer, intermediate (hidden) layers that perform convolutions, and an output layer.	Loss of information in deep networks Solutions: Creating shorter paths from early layers or joining layers in a feed-forward manner
Stochastic Neural Networks (SNNs)	Networks that use random variations or stochastic weights.	Maps inputs to probability distributions over outputs	Models are built using stochastic weights, adding a randomness factor to the network	Balancing between randomness and deterministic behavior in predictions
Recurrent Neural Networks (RNNs)	Networks equipped to process temporal or sequential information.	Recognizes time series or sequential data. Previous outputs serve as inputs in a series	Can maintain hidden states, making them suitable for sequences and time series	Vanishing gradient problem. Solutions: Use of LSTM and GRU variants
Feed-forward Networks (MLPs)	Networks where data flows in one direction from input to output without loops or feedback.	Commonly used for tasks where data is not sequential or temporal. Can handle a wide range of tasks	Organized in sequential layers including an input layer, hidden layers, and an output layer	Limited complexity due to absence of loops or feedback mechanisms
Deep Neural Networks (DNNs)	Evolved from ANNs, they use deep learning techniques and combine aspects of both ML and ANNs.	Used for complex tasks where high-level feature extraction from raw input is needed	Comprises three or multiple layers. The more data used, the more accurate the performance	Overfitting with too many parameters. Solutions: Regularization methods, dropout

2.3 Natural Language Processing

The structured data like images , genetic data, Electronic Health Record (EHR) can be easily understandable by ML algorithms after preprocessing but a significant part of clinical data is unstructured that exist in narrative form which cannot be directly processed by computers. Here comes the role of Natural Language processing which extracts the narrative information from physical examination, laboratory reports and aid in clinical decision making.

- **NLP Pipeline Components:** An NLP pipeline typically consists of two main components:

1. **Text Processing:** NLP identifies disease-relevant keywords in clinical notes based on historical databases.
2. **Classification:** Selected keywords are examined for their impact on classifying normal and abnormal cases. Validated keywords are then integrated into structured data to support clinical decision-making.

Study Authors	NLP Application	Outcome/Result
Fiszman et al	Reading chest X-ray reports	Assisting antibiotic system to alert physicians for potential anti-infective therapy.
Miller et al	Monitoring laboratory-based adverse effects	Automating the monitoring of adverse effects in laboratory data.
Castro et al	Identifying cerebral aneurysm-associated variables	Achieving high accuracy rates in classifying patients based on 14 disease-associated variables.
Afzal et al	Extracting peripheral arterial disease-related keywords	Achieving over 90% accuracy in classifying patients with peripheral arterial disease.

- **Applications of NLP in Healthcare**
  - Alerting timely treatment arrangements.
  - Monitoring adverse risk effects from narrative text such as in laboratory reports.
  - Assisting in disease diagnosis.
- **Challenges in NLP**

1. **Language Complexity:** Variations in language, including jargon, slang, idioms, and synonyms, can pose difficulties for NLP models in accurately understanding and processing text.
2. **Typos and Errors:** Text and speech data frequently contain typos, grammatical errors, and mispronunciations, which can challenge NLP's ability to handle and correct these issues.
3. **Data Privacy and Security:** Ensuring data privacy and security, particularly in sensitive domains like healthcare, is essential when using NLP techniques.
4. **Lack of Consensus:** Different industries may have varying terminology and definitions for the same concepts, making it challenging for NLP models to accurately interpret domain-specific information.

2.4 Fuzzy Logic

Fuzzy logic is a mathematical approach that was originally established by Plato and is an extension of Boolean logic, based on the mathematical theory of fuzzy sets. It was first introduced by Lotfi A. Zadeh, a computer science professor. It is used in decision making, pattern recognition, control system and characterization of transitional values between binary evaluations e.g. Instead of using crisp values like "too hot" or "too cold," fuzzy logic allows us to work with fuzzy sets that represent these conditions more flexibly like moderately hot, moderately cold etc. Fuzzy logic deals with a decision/outcome in graded or fuzzy manner and this ability of fuzzy logic to handle vagueness in data found it's application in various healthcare issues in more adaptive, responsive and human like manner to the actual situation in computer programming.

- Application of Fuzzy logic and it's components in healthcare are:-

Fuzzy Logic in Medicine: fuzzy logic enables healthcare professionals to make more informed and adaptive decisions by considering the gradations and uncertainties present in medical data include optimizing medication for HIV-positive patients, predicting coronary heart disease, managing medical waste, optimizing treatment decisions for diabetes patients. It found various applications in medical imaging, neurology (brain tissue analysis), radiology (improving radiation therapy decisions), oncology (cancer detection), dermatology (skin lesion classification), and epidemiology (studying fuzzy epidemics). It has also been utilized in nursing for decision-making.

Fuzzy linear programming (FLP)

FLP integrates conventional linear programming techniques with fuzzy logic to seek optimal solutions in scenarios characterized by vagueness or imprecision, offering decision-makers more adaptable choices. In the field of medicine, fuzzy linear programming has been employed in minimizing human productivity loss through the allocation of treatments to diverse disease populations. It has also been utilized in the development of balanced diet plans for individuals with eating disorders and disease-related lifestyles to optimize nutrient intake and daily nutritional requirements, ultimately resulting in well-balanced dietary plans.

Fuzzy Multiple-Criteria Decision Analysis (Fuzzy MCDA)

In the healthcare sector, where decision-making involves balancing multiple conflicting objectives, Multiple-Criteria Decision Analysis (MCDA) techniques are highly relevant. They enable the evaluation of healthcare options with consideration for various criteria, such as diagnostic and treatment devices, patient conditions, and hospital requirements. Fuzzy Multiple-Criteria Decision Analysis (Fuzzy MCDA) extends the capabilities of MCDA by incorporating fuzzy logic offers flexibility, allowing decision-makers to work with linguistic data and bounded continuous data, making it well-suited for complex medical scenarios. This combination of MCDA and fuzzy logic finds diverse applications in medicine, including cancer analysis (colon, liver, leukemia, pancreatic, lung, breast), HIV therapy alternatives, assessment of medical imaging devices, and optimization of medical device sterilization methods.

3. Applications of Biomedical intelligence tool in Biomedical sciences

BI is used in early detection and management of many diseases whose treatment is expensive and diagnosis is labour intensive. Many BI enabled computer tools and devices employed with various AI algorithms help for medical imaging, biomarker identification, illness progression, medical research. Thus BI in healthcare not only improve patient's lifestyle but help them to cope with it financially thus making it more economic.

Role of AI in various disciplines biological and medical sciences

3.1 AI in medical disease diagnosis and therapeutics

BI use to solve difficult healthcare problems and it can be used to analyze data from multiple chronic diseases mentioned below:-

3.1.1 AI in Alzheimer's disease

AD is a prevalent neurodegenerative disease with no known cure.It is characterized by the formation of neurofibrillary tangles and amyloid plaques in the brain. AD leads to dementia, which results in behavioral abnormalities, significant memory loss, and cognitive impairment.

AI help in effective Alzheimer's disease diagnosis and treatment by integrating data from patient's brain function through AI tools like EEGs for brain imaging ,PET scans for imaging physiological and biological function of brain, BCIs, MRI, SPECT that recognizes unusual changes in different regions of brain through which AI can predict the onset of AD , potential drug targets and discoveries of new drugs, uncover hidden correlations by understanding underlying biological mechanisms and anomalies.

3.1.2 AI in Diabetes

Diabetes is marked by elevated glucose level in blood due to inability of beta cells of pancreas to produce insulin or inability of cells to uptake insulin(insulin resistance). This could result in variety of anomalies such as neuropathy, nephropathy, retinopathy, and cardiomyopathy.

Diabetes management is brought by various AI tools like expert system, CAD. Intelligent sock named SenseGO detects pressure change on foot which is a risk factor for foot ulcers of diabetic patient. Peripheral diabetic neuropathy is diagnosed through an automated algorithm for extraction of morphometric parameters and phase shift analysis technique to view and classify corneal pictures. Microalbuminuria is a biomarker used to classify diabetic nephropathy in Type II diabetes patients detected through fuzzy classifier. Besides this, multiple logistic regressions, SVM classification and ML approaches used to anticipate diabetic nephropathy. CAD system is used for screening between diabetic retinopathy and normal digital images with some degree of sensitivity and specificity.

3.1.3 AI in Cancer detection

AI algorithms can analyze digital histopathology slides known as whole slide imaging (WSI) with precision, enhancing diagnosis of different malignant tumors.

In the realm of breast cancer, advanced tools like virtual mammography are enhancing early detection. CAD systems assist radiologists in pinpointing abnormalities in mammograms, especially in denser breast tissues. Innovative wearable technologies, such as the iTBra by

Cycardia Health, offer monthly breast scanning, monitoring temperature changes that might indicate cancer presence. The FDA-approved iReveal software predicts breast density, aiding in risk assessment. Curemetrix provides a unique "breast health score" for each image, further refining diagnosis. The G2SBC database integrates vital genetic data related to breast cancer, while artificial neural networks categorize images into cancerous and non-cancerous. Other AI tools predict patient survival times and assist in analyzing breast mass smears. In essence, AI is enhancing the accuracy, early detection, and personalized treatment strategies in breast cancer care.

AI development changed the conventional screening strategy for diagnosing cervical cancer by building and mining millions of clinical database of medical health record and pathological data. Thus these data are fetched to train AI models based on machine learning to built a prognostic model that could correctly denote the risk of post operative recurrance and death .

Artificial intelligence role in biochemistry

AI is used in biochemistry, a field of life sciences in the multi omics study, prediction of secondary structure of protein, studying protein and nucleic acid biochemistry, Immunotherapy, drug discovery and designing , predicting bioactivity and drug toxicity and enzyme engineering etc.

3.2.1 Multi omics study

Multi-Omics Data: The availability of multi-omics data, including genomics, transcriptomics, proteomics, and structural biology data finds vast application for AI in biology.

Genomics: ML tools have been developed for DNA sequence analysis, gene prediction, functional annotation, and mapping sequences .In Bioinformatics,the DNA sequence analysis on basis of alignment score is achieved through Basic Local Alignment Search Tool (BLAST).

Transcriptomics: Expressed Sequence Tag (EST) databases and the Sequence Read Archive (SRA) store raw data from transcriptomes, enabling the analysis of gene expression patterns.

Proteomics: To identify potential cancer biomarkers algorithms like Machine Learning and Neural Networks are used to detect Mass Spectrometry data of individual proteins.ML tools like "ML-ToF" aid in identifying amino acid sequences.

Interactomics: ML algorithms, including structure-based approaches like SpotON and Interactome INSIDER, are used to predict protein-protein interactions and hotspot residues involved in these interactions. They also provide information on mutations associated with diseases like cancer.

Systems Biology: ML is applied in systems biology to make models are derived from diverse omics sequencing data sources that identifies the binding sites for biomolecules of Central Dogmai.e. DNA, RNA & Proteins.

3.2.2 Protein Secondary structure prediction and development

Dynamic programming-based sequence alignment: It is the premier model for predicting the 2^0 protein structure. This method is particularly effective when a protein with an unknown 3D structure has sequence similarity with protein of a known 3D structure. In cases where there are no comparable sequences, secondary structure prediction techniques come into play. However, it's essential to approach with caution: using training data to test prediction accuracy can lead to misleadingly high success rates. The most accurate test is on a protein whose sequence isn't in the training set and bears no similarities.

Protein biochemistry: AI algorithms used to customize proteins sequences and models with improved stability, binding affinity, and immunogenicity. By target mining various disease related to multi-omics data. AI help scientists in identifying proteins and related biomolecules that could provide therapeutic solutions. Molecular dynamic simulations and Deep Learning help in development of functional and stable protein by predicting patterns of protein folding which aids Effectiveness of protein binding to it's specific target requires binding affinity prediction by use of AI models that estimate optimal binding affinities. AI trained on toxicological data predicts toxicity of protein structure and other biologics by analyzing structure-activity relationships(SAR). By leveraging patient data, disease characteristics, and treatment outcomes, AI algorithms predict patient responses and refine trial procedures by facilitating personalized treatment.

Nucleic Acid Biochemistry :AI models used in sequence analysis of diseased gene DNA/RNA and predicts deformities that arises due to defective gene functions thus help in designing gene based therapeutics. One such technique that is well known for target gene therapy is CRISPR/Cas9 technique which is efficient RNA guided target gene editing platform found naturally as part of bacterial immune system to protect them against invading bacteriophage/ plasmid .

Immunotherapy: AI tools and models are used to design therapeutic antibodies and vaccines and analyzing them for their potential in immunotherapy and vaccine efficiency like as in COVID 19 pandemics . Thus in pandemic, with the diverse clinical data several AI platforms helps to stratify patients based on their immunoprofiles and developed personalized immunotherapeutics.

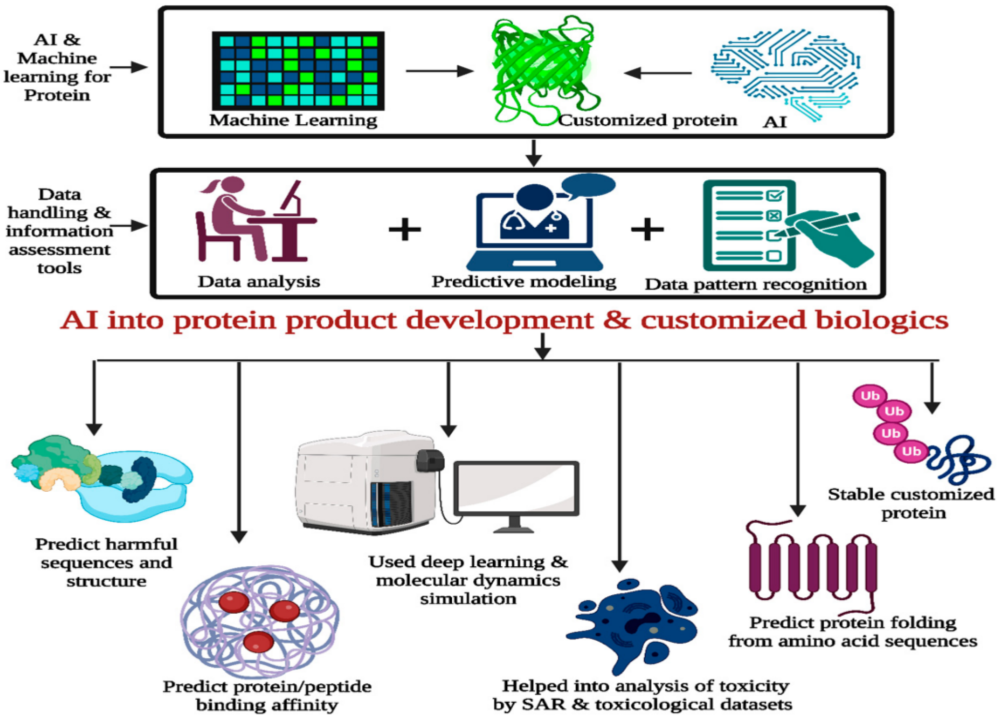

Figure 8: Role of ML in predictive modeling and development of customized protein

3.2.3 Drug discovery& Drug designing

As traditional methods take a long research time and constrained by high cost and absence of suitable technologies thus the introduction of AI MODELS in this domain could help in improvisation of drug development process. AI techniques, encompassing Machine Learning (ML), Deep Learning (DL), Expert systems & Artificial Neural Networks (ANNs), have revolutionized the drug discovery landscape, enhancing its efficiency.

AI adoption in drug discovery has transformed the process by making valuable contributions starting from target identification till toxicity prediction. In target identification AI system analyze various omics data and clinical data to understand molecular pathways and targets associated with disease. Virtual screening include screening of chemical spaces for simulating potential drug interaction with their targets based on binding affinities. QSAR (Quantitative structure activity relationship use to select drug based on certain activities like selectivity, potency, pharmacodynamics and pharmacokinetics. ML algorithms like reinforcement learning and generative modeling by learning from experimental data and chemical space for development of de novo drug design. Certain AI algorithms helps to optimize drugs based on their effectiveness, safety. Drug repurposing reduces cost and time in drug development by identifying potent role of existing drugs in theurapeutics. ML algorithms trained on toxicology databases identifies hazardous and harmful effect of chemicals prior to any clinical trial.

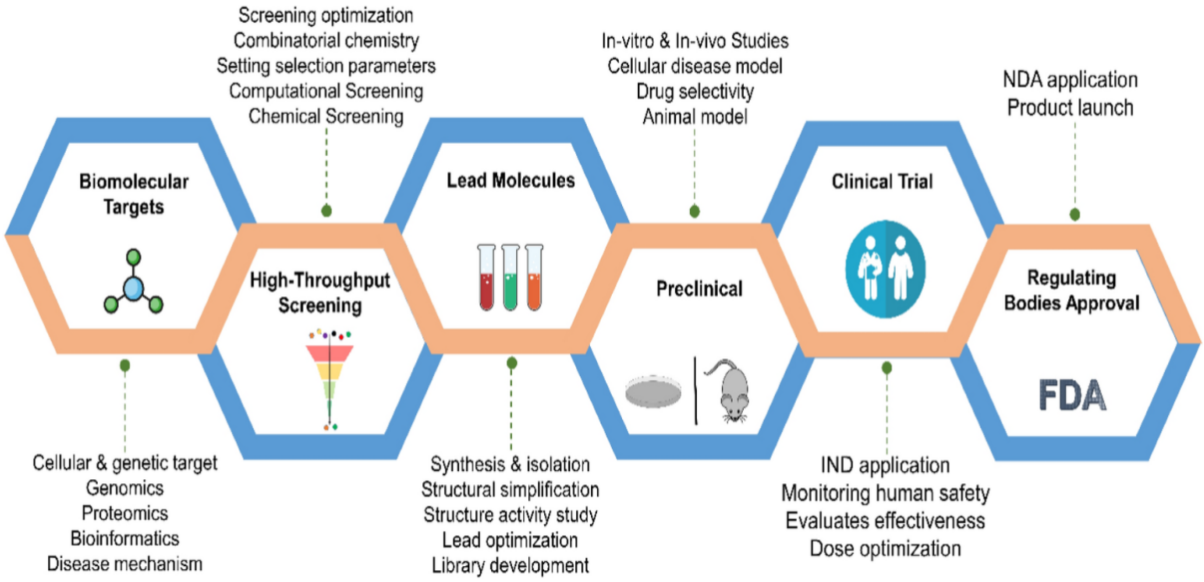

Figure 9: Highlights of Drug development process.

The table below shows the various AI-Aided Drug discovery tools used by different platforms with their applications:-

Companies/Platforms	AI Algorithms/Techniques Used	Application/Result
DeepChem	Deep learning models, virtual screening, generative chemistry	Molecular property prediction, virtual screening, generative chemistry in drug discovery
RDKit	Cheminformatics library	Molecule handling, substructure searching, descriptor calculation in drug discovery
ChemBERTa	Transformer-based language model	Molecular structure generation, property prediction, lead optimization in drug discovery
GraphConv	Deep learning on molecular graphs	Predicting molecular properties like bioactivity and toxicity
AutoDock Vina	Machine learning for binding affinity prediction	Virtual screening and lead optimization for drug discovery
SMILES Transformer	Deep learning model for SMILES strings	De novo drug design and lead optimization
Schrödinger Suite	Comprehensive software package with various AI-driven tools	Molecular modeling, virtual screening, drug design, and predictive modeling
IBM RXN for Chemistry	AI model for chemical reaction prediction	Predicting chemical reactions and discovering new synthetic routes
scape-DB	Database using NLP and machine learning	Extracting chemical and biological data from scientific literature for drug discovery

GENTRL	Generative tensorial reinforcement learning	De novo drug design and optimization of molecules with desired properties
DeepMind's AlphaFold	Deep neural networks (DNNs)	Predicts 3D protein structures, surpassing other algorithms; accurately predicted 25 out of 43 protein structures; winner of CASP13 protein-folding competition in Dec 2018
Insilico's GENTRL System	Generative adversarial networks (GANs) and other ML methods	Discovery of DDR1 kinase inhibitor; from target selection to active drug candidate in 46 days backed by in vivo data

In drug designing, various physical and chemical properties influence target receptor binding through molecular fingerprint and coulomb matriceswhich recognize molecule decriptors to predict binding properties .QSPR on other hand uses Estimation program intereface suits to study physiochemical property of drug. ADMET and ALGOPS program predicts lipophilicity and solubility based on Deep learning and Neural Network algorithms. These algorithms, combined with predictive models and in silico approaches, can predict the desired chemical structure of a compound. For instance, Pereira et al. developed DeepVS, a system that showcased impressive performance in docking a large number of receptors and ligands.

In drug discovery, AI use in analysis of Toxicity & Bioactivity of drugs which is summarized in the table given below:-

Technique/Platform	**Application/Description**
Chem Mapper	Predicts drug-target interactions
Deep Affinity	Deep learning method for predicting drug interactions; Not reliant on 3D protein structure
Online Tools	Helps in cutting down costs in drug development processes
Tox21 Data Challenge	Evaluates computational techniques for drug toxicity prediction
Deep Tox	Algorithm that uses static and dynamic features to predict toxicity

Thus in a nutshell, AI stremlining drug discovery pipelines from molecule prediction to drug design by leveraging vast databses, advanced algorithms and support the development of new therapeutics.

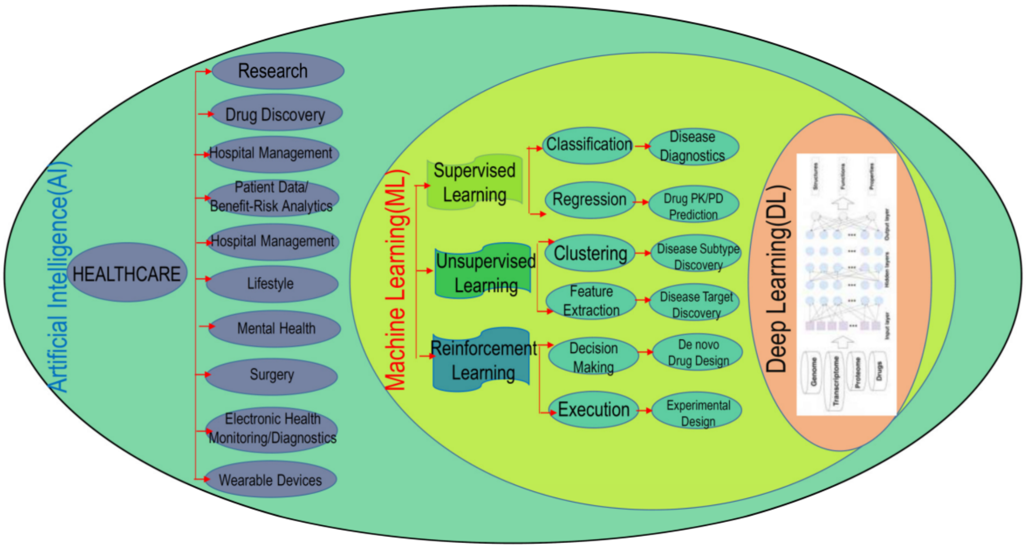

Figure 10: Hierarchy of AI algorithms used in drug discovery and development.

3.2.4 Enzyme Engineering

Machine learning (ML) is emerging as a valuable tool in enzyme engineering. ML predicts the structure based on a known sequence and vice versa, determining the substrate specificity or catalytic activity. ML plays crucial role in understanding how amino acid substitutions impact stability and solubility properties of enzymes which is essential for effective protein engineering.

While predicting protein structure has historically been challenging, deep neural networks, like AlphaFold, show promise in this area. Beyond structure prediction, determining catalytic activities is another focus. Various computational methods, ranging from sequence-based to genome-based, are employed. Initiatives like the Enzyme Function Initiative (EFI), COMBREX, and CAFA aim to enhance the functional annotation of enzymes. ML has been used to assign enzyme EC numbers, with deep learning recently being applied to predict EC numbers based on protein sequences. However, despite advancements, there are still challenges, especially in accurately predicting enzyme activity profiles due to their complexity.

4. Introduction to biomedical intelligence using Quantum computing

The coming together of two advanced fields, biomedical intelligence and quantum computing, is set to usher in a new era in understanding biology, improving healthcare, and speeding up scientific discoveries.

Biomedical intelligence, which uses smart computers, has made great strides in understanding how our bodies work, customizing medical treatments, and decoding our genes. However, dealing with a lot of complex medical data is challenging for regular computers. That's where quantum computers, which are incredibly powerful, can help.

Quantum computers excel at assisting with important medical research and healthcare challenges. They are different from regular computers and can study very tiny things like molecules and drugs with great precision. This can accelerate the discovery of new medicines and treatments.

Moreover, quantum computers can be used for various healthcare tasks, such as managing patient schedules, optimizing resource usage, and ensuring the security of healthcare information. They can even help create personalized treatments based on a person's unique genes and health history.

Many experts in healthcare and science are collaborating to harness the potential of quantum computers. They believe that combining the capabilities of quantum computers with the vast amount of medical data we have can revolutionize healthcare and research. In the future, we will gain a deeper understanding of how this works and the new opportunities it brings for a healthier and more informed world.

4.1 Quantum Computer Dedicated To Healthcare Research

The first super powerful quantum computer in a hospital was brought to Cleveland Clinic with the help of IBM. This project aims to speed up medical research using really fast computers and clever programs.

But regular hospitals can't buy these supercomputers because they're very expensive. For instance, a 50-qubit D-Wave One machine costs around $10 million, and it takes another million dollars each year to maintain it.

The CEO of Cleveland Clinic, Dr. Tom Mihaljevic, believes this technology can change healthcare and help find new treatments for diseases like cancer, Alzheimer's, and diabetes.

Cleveland Clinic plans to use the quantum computer for various research projects. They want to develop special programs for finding better drugs, predict the risk of heart problems after surgery, and find existing drugs that might help Alzheimer's patients.

They will also use the quantum computer to sort through a huge amount of medical data collected from patients. Smart sensors on bodies and at home generate a ton of data. Regular computers can't handle it all, but quantum computers can find new connections and process data from many patients at the same time, which could lead to new health discoveries.

Doctors will benefit too. Quantum computers can quickly analyze tons of medical information to diagnose rare diseases and figure out the best treatment based on individual patient data. This will help bridge the gap between medical research and real-world practice, as there's way too much medical information for doctors to keep up with. Quantum computers can do it in seconds.

4.2 Quantum Revolution?

Even though companies keep making better and better quantum computers, like IBM's latest one with 433 qubits, it will still be a few more years before lots of people can use this amazing technology.

One big issue is that the parts in these computers, called qubits, can sometimes make mistakes because they're not very stable. So scientists are working really hard to fix these mistakes.

Another problem is that there aren't enough scientists who know how to work with these supercomputers. Plus, they cost a lot of money, like tens of millions of dollars, and it's expensive to keep them running because they need super low temperatures.

But if they can make stable quantum computers, it could change medicine in a really big way.

5. Challenges In Integration of AI In Biomedical Domain

AI offers significant potential in biomedical sciences, addressing these technical, interpretability, data, ethical, and standardization challenges is essential for its successful integration and realization of its benefits in healthcare and research.

Explainable AI

Efforts are underway to develop more explainable AI models and methods to interpret DL algorithms. Techniques such as visualizing convolutional neural networks (CNNs) filters and using saliency and class activation maps aim to make DL models more interpretable.

Overfitting issues

The performance of machine learning (ML) algorithms is majorly dependent on the quantity and quality of input data. Overfitting can occur when models are trained on limited and noisy datasets. To improve AI algorithms, there is a need for larger and more diverse datasets, as well as careful data preprocessing and feature selection.

Sloppy data Integration:

There does not exist any validated method to accumulate and collate various diverse types of raw, unstructured, processed data , meta data etc which consequently affects output of ML algorithms , thus properly formatted data is crucial for integration into any AI algorithm.

Inadequate Data

AI models require substantial amounts of data for accurate predictions.Some drugs or populations may have inadequate data as a result the data used for training may not represent the target population, resulting in biased results or less accurate results.Rare diseases with limited data pose a significant challenge for AI model development.

Occupational and Skillset Immobility

Skills gap exists between data science, molecular chemistry, and biology. Many pharmaceutical professionals lack the necessary skills and qualifications to operate AI systems effectively. Bridging this gap is essential for creating relevant algorithms and leveraging AI effectively.

Proprietary and Black box AI Algorithms

Pharmaceutical companies often use proprietary AI algorithms that are not publicly accessible. Skepticism arises due to a lack of understanding of these "black box" as seen in Deep learning (DL) approaches, particularly deep neural networks and uncertainty about their results making it challenging to understand how they make predictions. This lack of transparency hampers model interpretability and limits their use, especially in clinical settings where transparency is crucial.

Complex Biological Systems

Biological systems involves numerous pathways, interconnected loops and Biomolecular interactions which poses heterogenity in data .Variability in result interpretation also arises due to genetic differences, environmental conditions etc. Thus, Lack of clear explanations for predictions makes it difficult for clinicians to understand and use AI models effectively.

Data Shortages in CV and Robotics: Computer vision (CV) and robotics applications in healthcare are limited by high-quality and diverse datasets. Additionally, these technologies require significant technical infrastructure and maintenance costs.

Inactive Molecules

AI simulations, such as docking algorithms for drug interaction with target may identify inactive molecules due to limitations in representing conformational flexibility and other factors. Experimental validation is essential for identification of molecular activity.

Standardization and Consensus

Lack of consensus poses challenges for NLP models. Establishing standardized vocabulary and further developing ontologies can help address this issue.

Inability to Incorporate New Data

AI models may struggle with incorporating new data or updates. In dynamic field like in drug development, the new information emerges constantly. Hence, updating AI models can be challenging and time-consuming failing which, can lead to inaccurate predictions and flawed decision-making. By integrating them into adaptable frameworks could be crucial to address this limitation.

Ethical Concerns

The increasing use of AI in healthcare raises ethical concerns related to patient's confidentiality, biases etc. In case of black box algorithm, there arises issue about liability, medical accountability and also cases of incorrect result predictions. Thus, thorough approval and authorized validation of data are essential to ensureefficiency, transparency and safety of AI tools.

Quantum Mechanics

Quantum mechanics is a big idea that helps us understand how things like matter and light act. In the world of quantum physics, things act a bit like waves. People used to think quantum mechanics only applied to super tiny things, but now they think it can help with tricky problems in areas like chemistry, physics, computer stuff, and making communication safer.

Quantum Theory

Quantum mechanics is a way of understanding things that happen in the quantum world. It tells us about a tiny particle's condition using something called a wave function, usually shown like this:

$\psi(x,t)$

The Schrödinger equation tells us how the wave function of the particle changes as time goes by, and it contains all the information about the particle.

$i\hbar\partial|\psi(t)\rangle\partial t=\hat{H}(t)|\psi(t)\rangle$.

In this equation, $\hbar$ stands for Planck's constant, and $\hat{H}(t)$ is like a special tool that tells us about the energy of the system.

Quantum Information Science:

Quantum information science has three main areas: quantum communication, quantum computing, and quantum sensing. Each area has its own specific research activities.

- Quantum Communication: This is about exchanging information on a quantum level. It includes things like quantum cryptography and networking, where people are finding new ways to keep information safe and share it using quantum principles.
- Quantum Sensing: Here, scientists are trying to make quantum devices work well with their surroundings. They're creating quantum systems and designs for different purposes.
- Quantum Computing: This is the third part. Quantum computers come in two types: analog and digital.
- Analog Quantum Computers: They run based on something called the system's Hamiltonian and the starting condition of qubits. There are three types:
- Adiabatic quantum computing (AQC): It uses a special kind of quantum process.
- Quantum annealing (QA): It's a way to find the best solution to a problem.
- Quantum simulation (QS): It helps us understand things that are tough to study with regular computers.
- Digital Quantum Computers: These work by doing specific operations, called gates, on qubits. Gate-based quantum computing is the most common type, and it's really important for things like quantum machine learning.

Quantum Computing System

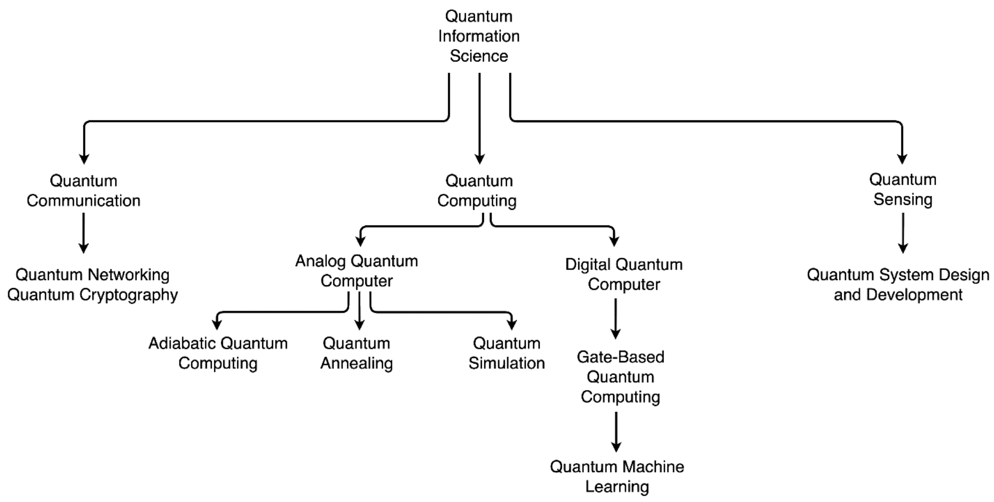

Figure 11:- Quantum information science (QIS) is like a big map with three main parts: quantum communication, quantum computing, and quantum sensing (and metrology).In quantum communication, we use quantum ideas to make cool things like quantum networking. For quantum sensing, it's all about designing special quantum systems. Now, when it comes to quantum computing, it's divided into two types: analog and digital. Analog quantum computers can be one of three types: adiabatic quantum computing, quantum annealing, or quantum simulation. But digital quantum computers work with something called gate-based quantum computing. It uses the power of QML for its operations.

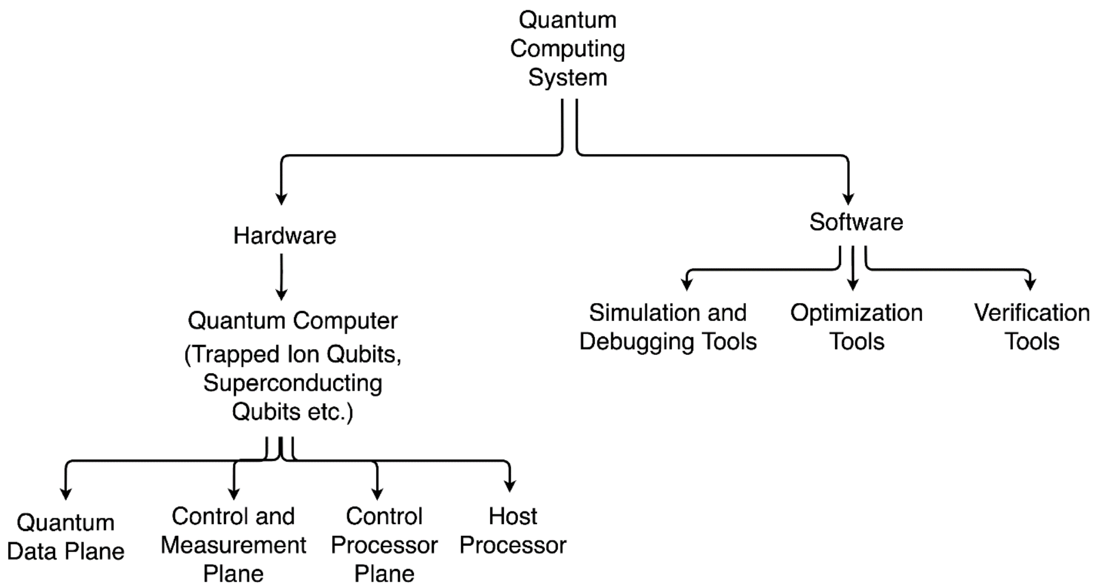

Figure 12: A Quantum Computing System (QCS) is like a whole package with two main parts: hardware and software. The hardware is like the computer itself, which has different types, such as trapped ion qubits and superconducting qubits. Inside a quantum computer, there are important parts like the quantum data part, the control and measurement part, the control processor part, and a host processor. The software is like the computer programs we use. In a QCS, you have tools like simulation and debugging tools, optimization tools, and verification tools to make the

computer work well. The hardware of a quantum system, the quantum computer, is made up of various components. The operation of these components necessitates the use of software tools. The various programming tools as they apply to a quantum system are visually represented in

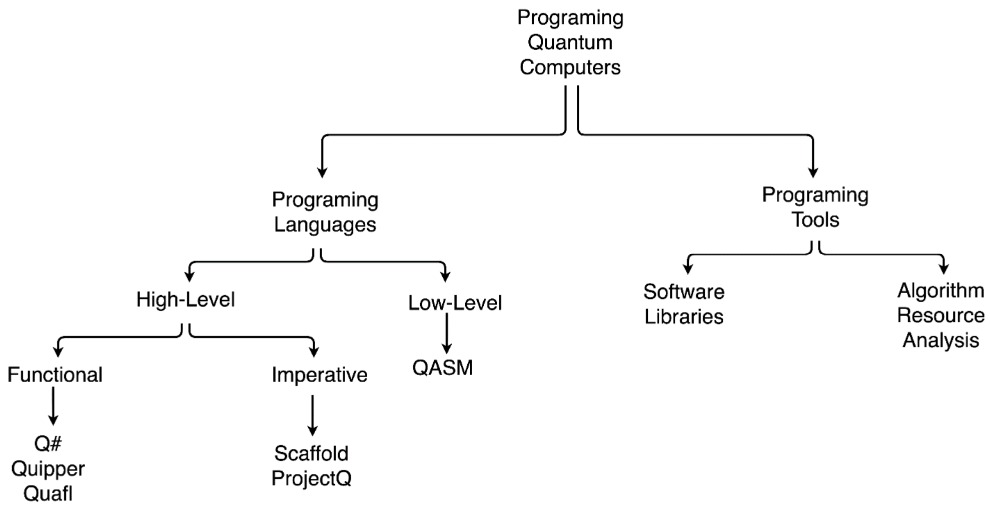

Figure: To make quantum computers work well, we need two important things: programming languages and programming tools. The programming language is like the way we talk to the computer. There are two types: low-level (like quantum assembly language) and high-level (like Quipper and ProjectQ), which makes it easier to give instructions to the computer.

Summary

This chapter unfolds how biomedical sciences have changed as a result of artificial intelligence (AI). The history of AI, which dates back to the 1920s, is covered at first, along with its several subtypes, such as Narrow AI and General AI.

Since the 1960s, when Dendral and MYCIN, two pioneering expert systems, were developed, AI has been transforming the biomedical sector. The Human Genome Project's completion in 2000 offered a wealth of data, advancing personalized medicine, medication discovery, and cancer research.

Today, AI aids in the analysis of medical data, improves resource allocation, and even enables real-time patient monitoring via gadgets like wearable sensors. To increase healthcare precision and safety, AI collaborates with surgical robots, biomedical imaging, and the Internet of Medical Things (IoMT).

Expanding healthcare access through telemedicine, it emphasizes technology and research for better patient care, particularly in tackling global health issues. In many medical domains, AI, particularly Machine Learning (ML) and Deep Learning (DL) drastically improved disease identification and patient treatment. Computers can now more easily comprehend medical writing thanks to natural language processing (NLP), which helps with disease diagnosis and side effect monitoring. Another AI strategy that aids in healthcare decision-making is fuzzy logic.

AI improves drug design, predicts drug activity, and expedites target identification in drug discovery. For stability, it is also helpful in enzyme engineering. But there are difficulties in integrating AI into healthcare, including the need to make it understandable, the need to work with sparse data, and ethical issues with accountability and privacy. Finally, AI holds the prospect of changing biomedical sciences.

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