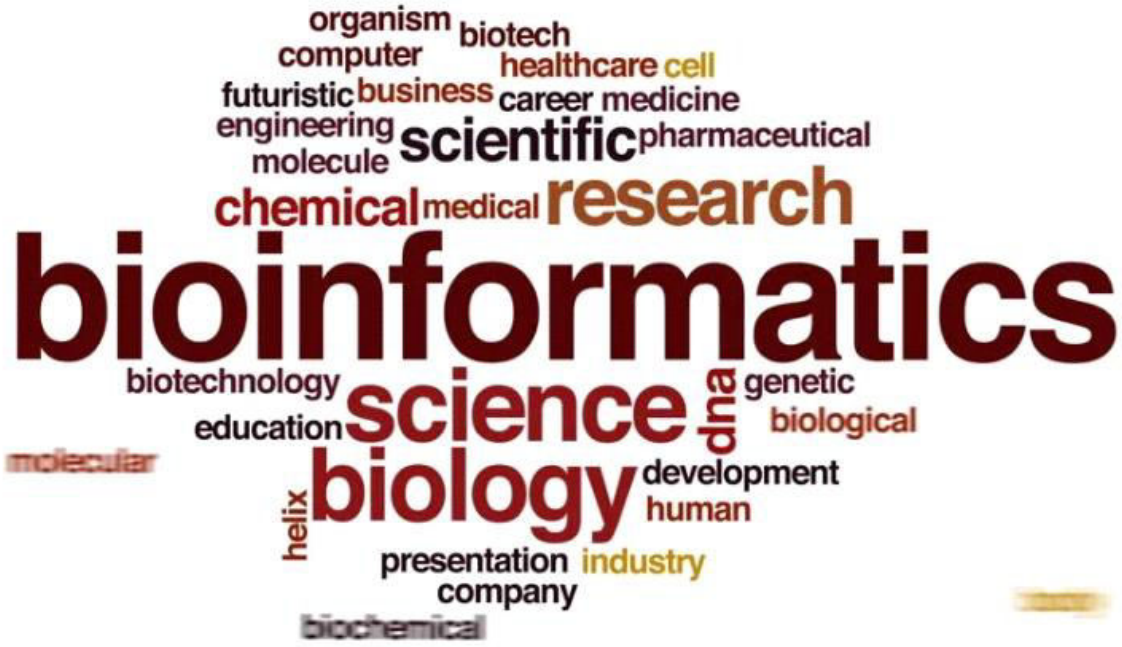
Unit-IV

Bioinformatics:



Bioinformatics is an interdisciplinary field that develops methods and software tools for understanding biological data. As an interdisciplinary field of science, bioinformatics combines biology, computer science, information engineering, mathematics and statistics to analyze and interpret biological data. Bioinformatics has been used for in silico (performed on computer or via computer simulation) analyses of biological queries using mathematical and statistical techniques.

Applications of Bioinformatics:

1. Analyze the biological processes.
2. Aids in improving drug discovery.
3. Help in developing new target drug.
4. Study and research.

Objectives of Bioinformatics:

The field of bioinformatics has three main objectives

- To organize vast reams of molecular biology data in an efficient manner
- To develop tools that aid in the analysis of such data
- To interpret the results accurately and meaningfully

Need for Bioinformatics:

- The need for Bioinformatics has arisen from the recent explosion of publicly available genomic information, such as that resulting from the Human Genome Project.
- Gain a better understanding of gene analysis, taxonomy, and evolution.
- To work efficiently on rational drug design and reduce drug development duration/time.

Bioinformatics Databases.

Databases are essential for bioinformatics research and applications. Many databases exist, covering various information types: for example, DNA and protein sequences, molecular structures, phenotype and biodiversity.

Databases may contain empirical data (obtained directly from experiments), predicted data (obtained from analysis), or, most commonly, both. They may be specific to a particular organism, pathway or molecule of interest.

Alternatively, they can incorporate data compiled from multiple other databases. These databases vary in their format, access mechanism, and whether they are public or not.

Some of the most commonly used databases are listed below:

- Used in biological sequence analysis: Genbank, UniProt
- Used in structure analysis: Protein Data Bank (PDB)
- Used in finding Protein Families and Motif Finding: InterPro, Pfam
- Used for Next Generation Sequencing: Sequence Read Archive
- Used in Network Analysis: Metabolic Pathway Databases (KEGG, BioCyc), Interaction Analysis Databases, Functional Networks
- Used in design of synthetic genetic circuits: GenoCAD
- Used in calculateion of drug DNA interaction: PREDDICTA

Classification of Bioinformatics Databases:-

Databases can be classified on the basis of:

a) Data type,

b) Data source,

c) Database design,

d) Special category.

Software and tools.

Software tools for bioinformatics range from simple command-line tools, to more complex graphical programs and standalone web-services available from various bioinformatics companies or public institutions.

Open-source bioinformatics software.

Many free and open-source software tools have existed and continued to grow since the 1980s. The combination of a continued need for new algorithms for the analysis of emerging types of biological readouts, the potential for innovative *in silico* experiments, and freely available open code bases have helped to create opportunities for all research groups to contribute to both bioinformatics and the range of open-source software available, regardless of their funding arrangements. The open source tools often act as incubators of ideas, or community-supported plug-ins in commercial applications.

The range of open-source software packages includes titles such as:

Bioconductor, BioPerl, Biopython, BioJava, BioJS, BioRuby, Bioclipse, EMBOSS, .NET Bio, Orange with its bioinformatics add-on, **Apache Taverna, UGENE and GenoCAD**.

Concept of Bioinformatics.

Bioinformatics is the application of computational technology to handle the rapidly growing repository of information related to molecular biology. ... It is particularly useful for managing and

analyzing large sets of data, such as those generated by the fields of genomics and proteomics.

Bioinformatics research and application include the analysis of molecular sequence and genomics data; genome annotation, gene/protein prediction, and expression profiling; molecular folding, modeling, and design; building biological networks; development of databases and data management systems; development of software.

Impact of Bioinformatics in Vaccine Discovery.

Vaccines are the pharmaceutical products that offer the best cost-benefit ratio in the pre- vention or treatment of diseases. In that a vaccine is a pharmaceutical product, vaccine development and production are costly and it takes years for this to be accomplished. Several approaches have been applied to reduce the times and costs of vaccine develop- ment, mainly focusing on the selection of appropriate antigens or antigenic structures, carriers, and adjuvants. One of these approaches is the incorporation of bioinformatics methods and analyses into vaccine development. This chapter provides an overview of the application of bioinformatics strategies in vaccine design and development, supply- ing some successful examples of vaccines in which bioinformatics has furnished a cutting edge in their development. Reverse vaccinology, immunoinformatics, and structural vac- cinology are described and addressed in the design and development of specific vaccines against infectious diseases caused by bacteria, viruses, and parasites. These include some emerging or re-emerging infectious diseases, as well as therapeutic vaccines to fight can- cer, allergies, and substance abuse, which have been facilitated and improved by using bioinformatics tools or which are under development based on bioinformatics strategies