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Bioinformatics: An emerging tool to address animal health

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Abstract

Bioinformatics has made a significant impact on biomedical research, playing crucial roles in structural and functional genomics, protein design and engineering, pharmaceutical development, animal genetics, ecology, veterinary medicine, and drug discovery. The primary tools employed by bioinformaticians include computer software programs and the internet. An illustrative example of bioinformaticians' value in veterinary and animal science is genome sequencing, which enhances animal health and production, thereby contributing to human nutrition and public health. In the long run, integrated bioinformatic analysis of genomic, pathological, and clinical data during clinical trials may unveil potential adverse drug reactions in individual animals, leading to personalized medicine through simple genetic tests and targeted therapies with minimal side effects. Advancements in bioinformatics have also furnished novel tools for identifying vaccine targets using sequenced biological data. This review aims to explore the significance and applications of bioinformatics in various fields of veterinary and animal sciences, paving the way for new avenues in veterinary research that ultimately benefit both animal and human health.

Keywords: Bioinformatics, Veterinary sciences, Vetinformatics

Introduction

In 1970, Paulien Hogeweg and Ben Hesper given the term "bioinformatics" to describe the study of informatic processes in biotic systems. Using information technology to manage biological data is known as bioinformatics. According to the National Centre for Biotechnology Information (NCBI 2001), bioinformatics is the interdisciplinary study of biology, computer science, and information technology. As the Human Genome Project (HGP) progressed, the amount of biological data increases marvellously and wonderfully (Wani *et al.*, 2018) [41]. The human genome sequence data is so large that, if it were collected into books, it would fill 200 volumes with 1000 pages each, and just reading it would take 26 years of nonstop work. The issue of managing such a large amount of data is only made possible by bioinformatics (Jhala *et al.*, 2011) [13]. Margaret Dayhoff, an American physical chemist who lived from 1925 to 1983 and made significant discoveries and employed computational methods in the study of biochemistry and protein sciences, was the first bioinformatician. The use of diverse bioinformatics tools in biological research facilitates the storage, retrieval, analysis, annotation, and visualisation of results and fosters a deeper comprehension of biological systems (Wani *et al.*, 2018) [41].

Role of Bioinformatics in Veterinary Sciences

In the field of veterinary science, the livestock production system is a complicated procedure with three interrelated fundamental elements: animal biology, the environment, and management strategies (Tiwary, 2022) [38]. Therefore, in order to increase cattle productivity and sustainability, vetinformatics approaches are needed to close the gaps between genotype and phenotype. In order to provide high-quality veterinary care for livestock animals, the idea of vetinformatics has been established as a subfield of bioinformatics (Sujatha *et al.*, 2018) [35].

Bioinformatics tools and algorithms have been developed as a result of the fast-expanding sequencing biological data. Using bioinformatics algorithms (tools), biological sequencing data is analysed. Bioinformatics' deals with certain objectives such as: First, data should be set up so that researchers can access the material already there and add new items as they are created. Second, to create resources and tools that help with data analysis. Thirdly, utilise a tool (or tools) to analyse the data and interpret the findings in a way that has biological significance. The fundamental local alignment search tool BLAST, FASTA, and Clustal W are a few of the frequently used bioinformatics tools. Using bioinformatics algorithms, such as BLAST (Basic Local Alignment Sequence Tool), FASTA and Clustal W solutions for sequence search and analysis, in combination with other techniques, constitutes a time- and money-efficient way to obtain crucial information on gene and protein levels that is difficult to obtain by other techniques (Kaikabo and Kalshingi, 2007) [16].

BLAST stands for Basic Local Alignment Search Tool, which is used for quick searches of protein and nucleotide databases (Altschul *et al.*, 1990) [2]. In order to provide useful biological information for the unidentified Sequence used for the search, it compares sequence data with the sequences that have already been characterised (Kaikabo and Kalshingi, 2007) [16]. Clustal W is a general-purpose method used for deoxyribonucleic acids (DNA) or protein multiple sequence analyses. It creates divergent sequence multiple sequence alignments that are biologically significant (Thompson *et al.*, 1994) [36]. The FASTA tool enables the comparison of a query sequence to a database of DNA sequences. The programme conducts a quick search to quickly locate database sequences that share a lot of similarities with the query sequence (Pearson and Lipman, 1988) [27].

Recent developments in the fields of molecular biology, particularly recombinant DNA technology, genomics, transcriptomics, metabolomics, and proteomics, which are sometimes also referred to as 'omics', have resulted in an enormous amount of data generation related to biological information that needs to be processed, managed, analysed, and stored (Khalid *et al.*, 2021) [17]. Recent advances in multi-omics platforms have generated an abundance of genetic and genomic data for livestock that must be transformed into information for breeding, disease prevention and control, productivity, and sustainability (Pathak and Kim, 2022) [26]. Virtually all of the next-generation omics technologies and techniques, such as genomics, transcriptomics, and proteomics, that are employed in other biological sciences disciplines can be used to veterinary science (Kadarmideen, 2014; Kaikabo and Kalshingi, 2007) [15, 16].

Bioinformatics nowadays is very fruitful in various veterinary related fields such as vaccine development, disease diagnosis, drug discovery, epidemiology, animal genetics, animal reproduction, animal nutrition etc. hence, it creates a vast field for various research and development approaches as well as beneficial for society.

Role of Bioinformatics in Vaccine Development, Disease Diagnosis and Drug Discovery: Emerging infections pose a serious danger to livestock productivity, necessitating the identification of potential vaccine candidates to guarantee long-term animal protection (Kaikabo and Kalshingi, 2007;

Ganguly *et al.*, 2013) [16, 9]. New approaches to vaccine development must be developed in order to offer broad-spectrum and long-term protection against various viral and bacterial illnesses (Pathak *et al.*, 2020; Gebre *et al.*, 2021) [25, 11]. Because bioinformatics has made it easier to identify vaccine targets from sequenced biological data of organisms, research and the production of future veterinary vaccines have both advanced as a result. The time and expense associated with Vaccinology have been significantly reduced by the use of bioinformatics in the discovery of vaccine targets (Kaikabo and Kalshingi, 2007) [16]. In order to create vaccines that offer defence against animal diseases, researchers can now make use of cutting-edge vetinformatics techniques (Kaikabo and Kalshingi, 2007; Mugunthan and Mani Chandra, 2021; Ganguly *et al.*, 2013) [16, 23, 9]. Thus, the development of naked DNA vaccines was made possible by the identification of target antigenic peptides in a genomic sequence of pathogens (Kaikabo and Kalshingi, 2007) [16].

Metabolomics can be used to determine predictors of inter-individual variability in drug response, give clinicians information to aid in drug selection decisions, and provide information on the pharmacokinetics and pharmacodynamics of a certain medication (Rivera-Velez *et al.*, 2021) [28]. By examining transcription start sites and promoter regions of bovine olfactory receptors using in silico analysis, the study discovered five candidate motifs (MOR1, MOR2, MOR3, MOR4, and MOR5) that are crucial for gene regulation (Samuel and Dinka, 2020) [30].

Both human and animal viruses have given rise to a plethora of bioinformatics tools that can help analyse genetic material related to the virus and design medically useful success plans that can avert disasters before they start. A hereditary information unit that is translated into a protein is called an open reading frame (ORF). Viral genome analysis is the method by which ORF is found. It serves as the foundation for additional study, including the search for similar structures or positions, the description of potential future events in proteins, functional analysis, therapeutic strategies to prevent viral diseases, and the identification of virus-killing targets (Latchman, 2005) [20]. Bioinformatics may be utilised to pinpoint diagnostic issues and come up with creative answers for the ongoing development and enhancement of molecular diagnostics (Kaikabo and Kalshingi, 2007) [16]. Similar to Kumar (2003) [19], who employed bioinformatics to find antigenic epitopes from the Rabies virus glycoprotein G that might be exploited for the creation of an anti-rabies subunit vaccine.

Molecular Docking: Recent advances in computational methods have aided in the optimisation of lead compounds, the prediction of pharmacokinetics and pharmacodynamics, and the calculation of receptor-ligand binding energy through molecular docking simulations (Verma and Pathak, 2022) [40]. Arya *et al.* (2023) [3] conducted an *In-silico* study comparing the antibacterial activity of Tulsi and Garlic against *S. aureus* and *E. coli* using molecular docking in the direction to find potent antibacterial agent.

Compounds can be retrieved from databases such as ZINC which can fulfill pharmacokinetic criteria and can be selected for drug designing and vaccine development using protein modeling, epitope prediction, and molecular docking of the target proteins for *e.g.*, target proteins of *Brucella i.e.*, BvrR, OMP25, and OMP31 and can be considered as lead

molecules for potentially inhibiting *Brucella's* proteins (Elrashedy *et al.*, 2024) ^[10]. *Macleaya cordata* (Willd.) was found to have multi-component synergistic mechanism of action in the treatment of bovine hoof disease which was analysed using bioinformatics-based network topology strategy and molecular docking study and upon visual network analysis it was found that the four active compounds, sanguinarine, chelerythrine, allocryptopine and protopine of the plant were associated with the 10 target genes/proteins (SRC, MAPK3, MTOR, ESR1, PIK3CA, BCL2L1, JAK2, GSK3B, MAPK1, and AR) (Dong *et al.*, 2021) ^[4]. Bioinformatic sequence comparison methods can be used to identify potential target proteins in some parasitic nematodes and arthropods on expressed sequence tags and S-adenosyl-l-methionine synthetase was characterized as interest target protein which can help in the development of new drug candidates (Krasky *et al.*, 2007) ^[46]. Network pharmacology can also be used to explore the mechanism of the control of poultry coccidiosis using modified gegen qinlian decoction after finding the target genes and then using the molecular docking to find the extent of binding of the key target genes (Peng *et al.*, 2022) ^[29]. Computational methods were used to identify the potential inhibitors targeting the LSDV-encoded DNA polymerase protein (gene LSDV039) and it was found that taxifolin had superior stability and binding energy and helped in LSD therapeutics (Zia *et al.*, 2024) ^[31].

Simulation of proteins and protein-ligand interactions using molecular dynamics: The movement and behaviour of a molecular system at the atomic level can be computationally visualised using molecular dynamics simulation (Singh and Pathak, 2020; Tiwari and Singh, 2022) ^[33, 37]. It provides intricate structural details on macromolecular structures and a plethora of knowledge about the interactions between proteins and ligands (Pathak *et al.*, 2020; Singh and Pathak, 2020) ^[25, 33]. This information is essential for comprehending the target's structure–function relationship and its dynamics during interactions with proteins and ligands, which will ultimately aid in the development of new drugs (Pathak *et al.*, 2020) ^[25]. Molecular dynamics (MD) simulations validate docking results, as demonstrated by Tyagi *et al.* (2018) ^[45] in determining the activity of MMV019838 on Mtb. In another study, Sharma *et al.* (2023) ^[44] conducted an *in-silico* study that showed good binding energy and strong hydrogen bond in docking of MMV675968 with ec-DHFR. Molecular dynamic studies further validated this finding, that revealed high binding free energy in ec-DHFR.

Role of Bioinformatics in Animal Genetics: The field of bioinformatics creates and offers techniques and resources to assist biologists in identifying genuine signals, which are biological activity expressions mixed together in a large data set. Veterinary science utilises tools and techniques from the field of bioinformatics to enhance cattle breeds by utilising huge biological datasets to comprehend the systems genetics of complex traits (Kadarmideen, 2014) ^[15]. In order to identify functionally linked features that may contribute to genetic diversity, it is also helpful to detect different sequence variants, such as single nucleotide polymorphisms, copy number variations, insertions, and deletions (Daetwyler *et al.*, 2013) ^[7]. A growing need for food in the livestock industry necessitates improved production Animal heredity is studied by animal genetics. People questioned

how some diseases are passed down through the centuries, why children look like their parents, and what keeps them unique. The idea that genes are passed down regularly through generations was originally recognised by Mendel. Presently, science knows that DNA molecules carrying sequences of four nucleotides (A, T, G, and C) are passed down from one generation to the next. The genome, the blueprint for all biological structures and functions, contains whole sequence information of an organism. The study of the genome is known as genomics (Cooper, 1994) ^[5]. It looks at the molecular data to comprehend disorders and natural variation. Large data sets, spanning terabytes, are produced by DNA sequencing and alignment, gene expression measurement techniques, and more intricate modelling studies like protein folding patterns. These sets would be impossible to analyse and interpret without the use of contemporary computational and machine learning capabilities. To properly apply such analytical techniques to the study of biological systems, one must possess mathematical and statistical expertise.

To sequence the genome of domestic cow (*Bostaurus*), Zimin *et al.* (2009) ^[43] combined whole-genome shotgun sequencing and hierarchical sequencing methods (Zimin *et al.*, 2009) ^[43]. Using sequence alignment and analysis, Ajayi *et al.* discovered 67 genes in the bovine genome that are members of heat shock protein families (Ajayi *et al.*, 2018) ^[1]. In pigs affected by mycoplasma pneumonia of swine, Uemoto *et al.* (2021) ^[39] used GWAS (Genome-Wide Association Studies) to identify six significant quantitative trait loci for immune-related features, providing new insights into the genetic factors affecting pig production, respiratory illness, and immune-related qualities (Uemoto *et al.*, 2021) ^[39]. Another GWAS-based analysis found candidate genes for individual birth weight features in Korean Yorkshire piglets and milk production variables in Korean Holstein cattle (Kim *et al.*, 2021; Lee *et al.*, 2020) ^[18, 21]. Therefore, GWAS-based methods have the potential to unravel crucial and intricate features connected to cattle productivity (Pathak and Kim., 2022) ^[26].

Role of Bioinformatics in Animal Reproduction: By comprehending the interactions of the protein responsible for reproduction between chemical modulators and medicinal molecules, bioinformatics plays a crucial part in the reproductive sciences research (D'Cruz *et al.* 2012) ^[6]. Animal breeders therefore rely on the use of various databases, including genetic control databases (GDC), for the early detection of potential inherited disease carriers as well as for examining and separating the genotypes into affected, carriers, and normal which would prove to be beneficial for their experimental studies (Jovanović *et al.*, 2009) ^[14]. Various bioinformatics techniques, including transcriptome analysis, genome annotation, microarray data analysis, genome-wide association studies, protein structure prediction, phylogenetic analysis, and genetic diversity analysis, assist breeders in increasing livestock production by selecting animals with improved and desirable traits and by breeding animals with disease resistance traits (Singh *et al.*, 2018) ^[34]. Porcine ovaries' RNA-Seq study of differentially expressed genes indicated 4,414 of these genes' functions in the late metestrus and diestrus phases of the estrous cycle (Park *et al.*, 2022) ^[24].

Role of Bioinformatics in Animal Nutrition: In animal nutrition studies, the use of metabolomic analysis is primarily limited to determining how dietary elements affect the metabolome of certain organs or tissues. Bioinformatics aids researchers in identifying the target region in the genomes of Rumen microorganisms and forecasting the effects of metabolomics on genes and their proteins. Therefore, bioinformatics techniques can also be used to identify changes in the biochemical profiles of the plasma and urine of experimental animals. In order to increase animal productivity and general performance, bioinformatics techniques such as DAVID (The Database for Annotation, Visualization and Integrated Discovery) are perfect for methodically extracting biological meaning from vast gene/protein lists and helping find specific indicators for manipulating gene expression through the use of nutrients or their combinations (Mathur and Kumar, 2018) [22].

Future considerations

Computer-based analyses of livestock data require veterinary science-related databases and technologies (Sujatha *et al.*, 2018) [35]. A few animal-specific databases have been created recently as a result of advancements in the field of vetinformatics; however, the availability of these databases is still lacking (Dawson *et al.*, 2017; Shamimuzzaman *et al.*, 2020; Yang *et al.*, 2020) [8, 32, 42]. Large multi-omics data sets about farm animals are desperately needed in the post-genomic era to create species-specific databases that will aid veterinary research. Furthermore, multi-omics data will be made available to enhance the forecast, creation, and precision of novel algorithms that address issues with animal breeding, create disease diagnostics, and provide solutions that boost livestock productivity and sustainability (Greener *et al.*, 2022) [12].

Conclusion

Techniques in veterinary informatics have demonstrated their capacity to address a wide range of issues in veterinary research. Vetinformatics is becoming an important topic and a well-liked multidisciplinary study area in the veterinary sciences. This review emphasised the power of vetinformatics and how its approaches can be applied to difficult veterinary science undertakings.

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