

A Computational Method for Sequence analyzing

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Abstract: To study how normal cellular activities are altered in different disease states, the biological data must be combined to form a comprehensive picture of these activities. Therefore, the field of bioinformatics has evolved such that the most pressing task now involves the analysis and interpretation of various types of data. This includes nucleotide and amino acid sequences, protein domains, and protein structures. Common uses of bioinformatics include the identification of candidate genes and nucleotides (SNPs). Often, such identification is made with the aim of better understanding the genetic basis of disease, unique adaptations, desirable properties (esp. in agricultural species), or differences between populations. In a less formal way, bioinformatics also tries to understand the organisational principles within nucleic acid and protein sequences.

Keywords: Clustering, RNA sequences, RNA-Seq, Data Mining, Bioinformatics, Graph Mining.

1. INTRODUCTION

Bioinformatics has become an important part of many areas of biology. In experimental molecular biology, bioinformatics techniques such as image and signal processing allow extraction of useful results from large amounts of raw data. In the field of genetics and genomics, it aids in sequencing and annotating genomes and their observed mutations. It plays a role in the text mining of biological literature and the development of biological and gene ontologies to organize and query biological data. It also plays a role in the analysis of gene and protein expression and regulation. Bioinformatics tools aid in the comparison of genetic and genomic data and more generally in the understanding of evolutionary aspects of molecular biology. At a more integrative level, it helps analyze and catalogue the biological pathways and networks that are an important part of systems biology. In structural biology, it aids in the simulation and modeling of DNA, RNA, and protein structures as well as molecular interactions.

Sequences

Computers became essential in molecular biology when protein sequences became available after Frederick Sanger determined the sequence of insulin in the early 1950s. Comparing multiple sequences manually turned out to be impractical. A pioneer in the field was Margaret Oakley Dayhoff, who has been hailed by David Lipman, director of the National Center for Biotechnology Information, as the "mother and father of bioinformatics" [1-10] Dayhoff compiled one of the first protein sequence databases, initially published as books [2] and pioneered methods of sequence alignment and molecular evolution [3] Another early contributor to bioinformatics was Elvin A. Kabat, who pioneered biological sequence analysis in 1970 with his comprehensive volumes of antibody sequences released with Tai Te Wu between 1980 and 1991.

Genomes

As whole genome sequences became available, again with the pioneering work of Frederick Sanger [4-15] it became evident that computer-assisted analysis would be insightful. The first analysis of this type, which had important input from cryptologists at the National Security Agency, was applied to the nucleotide sequences of the bacteriophages MS2

and PhiX174. As a proof of principle, this work showed that standard methods of cryptology could reveal intrinsic features of the genetic code such as the codon length and the reading frame. This work seems to have been ahead of its time—it was rejected for publication by numerous standard journals and finally found a home in the *Journal of Theoretical Biology*. [9-25] The term bioinformatics was re-discovered and used to refer to the creation of databases such as GenBank in 1982. With public availability of data, tools for their analysis were quickly developed and described in journals, such as *Nucleic Acids Research*, which published specialized issues on bioinformatics tools as early as 1982.

To study how normal cellular activities are altered in different disease states, the biological data must be combined to form a comprehensive picture of these activities. Therefore, the field of bioinformatics has evolved such that the most pressing task now involves the analysis and interpretation of various types of data. This includes nucleotide and amino acid sequences, protein domains, and protein structures.[25-35] The actual process of analyzing and interpreting data is referred to as computational biology. Important sub-disciplines within bioinformatics and computational biology include:

Development and implementation of computer programs that enable efficient access to, use and management of, various types of information

Development of new algorithms (mathematical formulas) and statistical measures that assess relationships among members of large data sets. For example, there are methods to locate a gene within a sequence, to predict protein structure and/or function, and to cluster protein sequences into families of related sequences.

The primary goal of bioinformatics is to increase the understanding of biological processes. What sets it apart from other approaches, however, is its focus on developing and applying computationally intensive techniques to achieve this goal. Examples include: pattern recognition, data mining, machine learning algorithms, and visualization. Major research efforts in the field include sequence alignment, gene finding, genome assembly, drug design, drug discovery, protein structure alignment, protein structure prediction, prediction of gene expression and protein–protein interactions, genome-wide association studies, and the modeling of evolution. Bioinformatics now entails the creation and advancement of databases, algorithms, computational and statistical techniques, and theory to solve formal and practical problems arising from the management and analysis of biological data. Over the past few decades rapid developments in genomic and other molecular research technologies and developments in information technologies have combined to produce a tremendous amount of information related to molecular biology. Bioinformatics is the name given to these mathematical and computing approaches used to glean understanding of biological processes.

2. SEQUENCE ANALYSIS

Since the Phage Φ -X174 was sequenced in 1977,[11] the DNA sequences of thousands of organisms have been decoded and stored in databases. This sequence information is analyzed to determine genes that encode proteins, RNA genes, regulatory sequences, structural motifs, and repetitive sequences. A comparison of genes within a species or between different species can show similarities between protein functions, or relations between species (the use of molecular systematics to construct phylogenetic trees). With the growing amount of data, it long ago became impractical to analyze DNA sequences manually. Today, computer programs such as BLAST are used daily to search sequences from more than 260 000 organisms, containing over 190 billion nucleotides.[35-47] These programs can compensate for mutations (exchanged, deleted or inserted bases) in the DNA sequence, to identify sequences that are related, but not identical. A variant of this sequence alignment is used in the sequencing process itself. The so-called shotgun sequencing technique (which was used, for example, by The Institute for Genomic Research to sequence the first bacterial genome, *Haemophilus influenzae*)[13] does not produce entire chromosomes. Instead it generates the sequences of many thousands of small DNA fragments (ranging from 35 to 900 nucleotides long, depending on the sequencing technology). The ends of these fragments overlap and, when aligned properly by a genome assembly program, can be used to reconstruct the complete genome. Shotgun sequencing yields sequence data quickly, but the task of assembling the fragments can be quite complicated for larger genomes. For a genome as large as the human genome, it may take many days of CPU time on large-memory, multiprocessor computers to assemble the fragments, and the resulting assembly usually contains numerous gaps that must be filled in later. Shotgun sequencing is the method of choice for virtually all genomes sequenced today, and genome assembly algorithms are a critical area of bioinformatics research [48-59] Figure 1 shows an overview of our aligned sequences

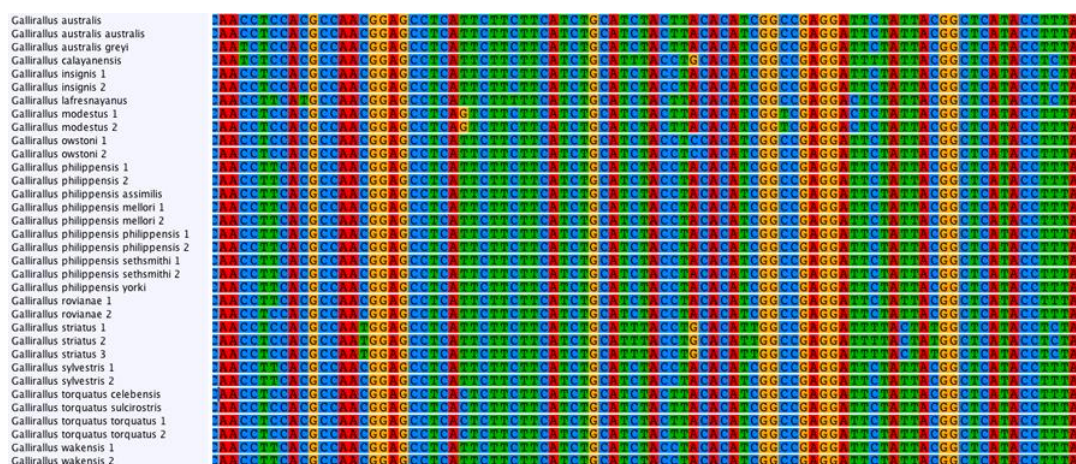


Figure1. an overview of our aligned sequences

Another aspect of bioinformatics in sequence analysis is annotation. This involves computational gene finding to search for protein-coding genes, RNA genes, and other functional sequences within a genome. Not all of the nucleotides within a genome are part of genes. Within the genomes of higher organisms, large parts of the DNA do not serve any obvious purpose [36, 37, 38, 39, 40]. This so-called junk DNA may, however, contain unrecognized functional elements. Bioinformatics helps to bridge the gap between genome and proteome projects — for example, in the use of DNA sequences for protein identification.

Genome annotation

In the context of genomics, annotation is the process of marking the genes and other biological features in a DNA sequence. This process needs to be automated because most genomes are too large to annotate by hand, not to mention the desire to annotate as many genomes as possible, as the rate of sequencing has ceased to pose a bottleneck. Annotation is made possible by the fact that genes have recognisable start and stop regions, although the exact sequence found in these regions can vary between genes [80-95].

The first genome annotation software system was designed in 1995 by Owen White, who was part of the team at The Institute for Genomic Research that sequenced and analyzed the first genome of a free-living organism to be decoded, the bacterium *Haemophilus influenzae*. White built a software system to find the genes (fragments of genomic sequence that encode proteins), the transfer RNAs, and to make initial assignments of function to those genes. Most current genome annotation systems work similarly, but the programs available for analysis of genomic DNA, such as the GeneMark program trained and used to find protein-coding genes in *Haemophilus influenzae*, are constantly changing and improving.

Computational evolutionary biology

Evolutionary biology is the study of the origin and descent of species, as well as their change over time. Informatics has assisted evolutionary biologists by enabling researchers to:

trace the evolution of a large number of organisms by measuring changes in their DNA, rather than through physical taxonomy or physiological observations alone, more recently, compare entire genomes, which permits the study of more complex evolutionary events, such as gene duplication, horizontal gene transfer, and the prediction of factors important in bacterial speciation, build complex computational models of populations to predict the outcome of the system over time[14, 40, 41, 42, 43, 44]

track and share information on an increasingly large number of species and organisms Future work endeavours to reconstruct the now more complex tree of life. The area of research within computer science that uses genetic algorithms is sometimes confused with computational evolutionary biology, but the two areas are not necessarily related [60-79].

Comparative genomics

The core of comparative genome analysis is the establishment of the correspondence between genes (orthology analysis) or other genomic features in different organisms. It is these intergenomic maps that make it possible to trace the evolutionary processes responsible for the divergence of two genomes. A multitude of evolutionary events acting at

various organizational levels shape genome evolution. At the lowest level, point mutations affect individual nucleotides [31, 32, 33, 34, 35]. At a higher level, large chromosomal segments undergo duplication, lateral transfer, inversion, transposition, deletion and insertion. Ultimately, whole genomes are involved in processes of hybridization, polyploidization and endosymbiosis, often leading to rapid speciation [119-129]. The complexity of genome evolution poses many exciting challenges to developers of mathematical models and algorithms, who have recourse to a spectra of algorithmic, statistical and mathematical techniques, ranging from exact, heuristics, fixed parameter and approximation algorithms for problems based on parsimony models to Markov Chain Monte Carlo algorithms for Bayesian analysis of problems based on probabilistic models.

Many of these studies are based on the homology detection and protein families computation.

3. New METHOD

Tens of thousands of three-dimensional protein structures have been determined by X-ray crystallography and protein nuclear magnetic resonance spectroscopy (protein NMR) and a central question in structural bioinformatics is whether it is practical to predict possible protein–protein interactions only based on these 3D shapes, without performing protein–protein interaction experiments. A variety of methods have been developed to tackle the protein–protein docking problem, though it seems that there is still much work to be done in this field [15, 16, 17, 18].

Other interactions encountered in the field include Protein–ligand (including drug) and protein–peptide. Molecular dynamic simulation of movement of atoms about rotatable bonds is the fundamental principle behind computational algorithms, termed docking algorithms, for studying molecular interactions [130-150]. Clustering algorithms can be categorized based on their cluster model, as listed above. The following overview will only list the most prominent examples of clustering algorithms, as there are possibly over 100 published clustering algorithms. Not all provide models for their clusters and can thus not easily be categorized [98-118, 151].

There is no objectively "correct" clustering algorithm, but as it was noted, "clustering is in the eye of the beholder" [84]. The most appropriate clustering algorithm for a particular problem often needs to be chosen experimentally, unless there is a mathematical reason to prefer one cluster model over another. It should be noted that an algorithm that is designed for one kind of model has no chance on a data set that contains a radically different kind of model. For example, k-means cannot find non-convex clusters [19, 20, 21, 22, 23]. 20 clusters extracted, most of which contain single elements, since linkage clustering does not have a notion of "noise". Many people used this method on the different. K-means has a number of interesting theoretical properties. On the one hand, it partitions the data space into a structure known as a Voronoi diagram. On the other hand, it is conceptually close to nearest neighbor classification, and as such is popular in machine learning [27, 28, 29, 30]. Third, it can be seen as a variation of model based classification, and Lloyd's algorithm as a variation of the Expectation-maximization algorithm for this model discussed below (figure 2).

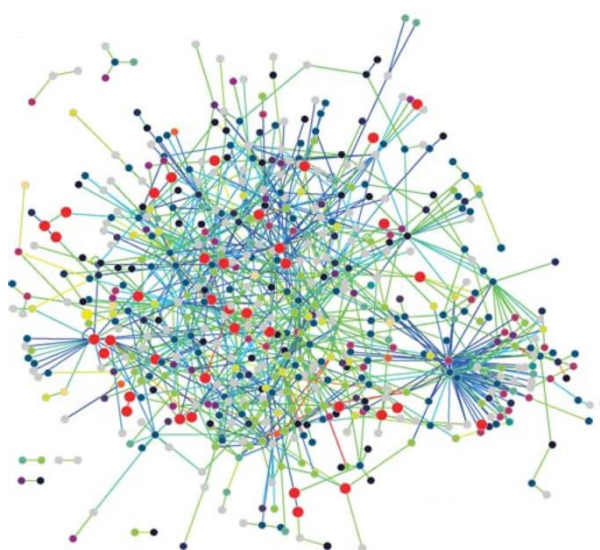


Figure2. Interactions between proteins are frequently visualized and analyzed using networks

Distribution-based clustering produces complex models for clusters that can capture correlation and dependence between attributes. However, these algorithms put an extra burden on the user: for many real data sets, there may be no concisely defined mathematical model (figure 3). Many people used this method on the different application [24, 25, 26, 27].

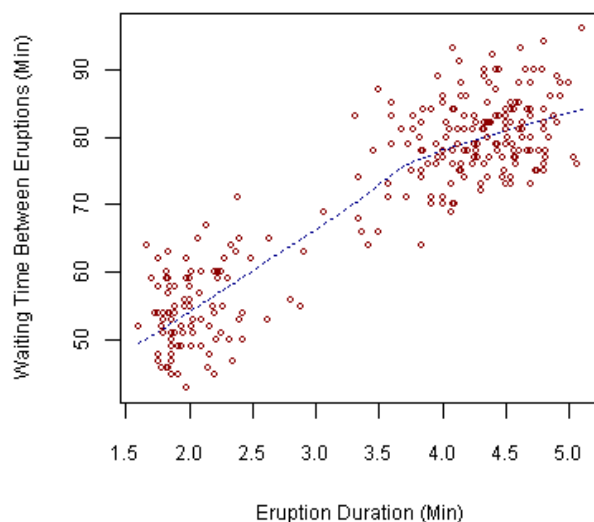


Figure3. A numerical solution to the heat equation on a pump casing model using the finite element method

Mean-shift is a clustering approach where each object is moved to the densest area in its vicinity, based on kernel density estimation. Eventually, objects converge to local maxima of density. Similar to k-means clustering, these "density attractors" can serve as representatives for the data set, but mean-shift can detect arbitrary-shaped clusters similar to DBSCAN. Due to the expensive iterative procedure and density estimation, mean-shift is usually slower than DBSCAN or k-Means.

6. CONCLUSION

Generally, data mining (sometimes called data or knowledge discovery) is the process of analyzing data from different perspectives and summarizing it into useful information - information that can be used to increase revenue, cuts costs, or both. Data mining software is one of a number of analytical tools for analyzing data. In simpler Markov models (like a Markov chain), the state is directly visible to the observer, and therefore the state transition probabilities are the only parameters. In a hidden Markov model, the state is not directly visible, but output, dependent on the state, is visible. Each state has a probability distribution over the possible output tokens. Therefore the sequence of tokens generated by an HMM gives some information about the sequence of states. Note that the adjective 'hidden' refers to the state sequence through which the model passes, not to the parameters of the model; the model is still referred to as a 'hidden' Markov model even if these parameters are known exactly. We proposed a fuzzy HMM for Data Mining, which applied on several applications. Our results showed that our proposed method is better than current methods.

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