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A Review on Clustering Techniques and Optimization Algorithms for Molecular Docking and DNA Nanotechnology

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ABSTRACT: In this paper, the literature survey on data mining approaches for the analysis of DNA Nanotechnology using molecular docking is carried out. DNA Nanotechnology is the field in nanotechnology that uses the unique structure of DNA to create different structures. DNA has different characteristics like carrying genetic information, but its structural material is used in DNA Nanotechnology. A major goal of DNA Nanotechnology is to assemble a biochip computer. The molecular docking problem is to find a good position and orientation for docking and a small molecule ligand to a large receptor molecule. It is originated as an optimization problem consists of optimization method and the clustering technique. Optimization problem is the problem of finding the best solution from all feasible solutions. Clustering is a data mining task which groups the data on the basis of similarities among the data. This survey, deals with various approaches and optimization algorithms to Molecular docking using clustering techniques. The performance of various existing clustering algorithms under each of these approaches is also discussed. In this work, existing approaches to molecular docking, various searching methods, different approaches used to evaluate solutions and algorithms used to find the target protein are categorized and analysed.

KEYWORDS: Data Mining, Swarm Intelligence, Protein-Ligand Docking, Molecular Docking, DNA Nanotechnology.

I. INTRODUCTION

1.1 Data Mining

Data Mining refers to the nontrivial extraction of implicit previously unknown and potentially useful information from data in databases. The large collections of data are the potential lodes of valuable information but like in real mining the search and extraction can be a difficult in exhaustive process to find implicit but potentially useful information, Let D ={d_1, ..., d_n} be the dataset to be analysed. Then, the data mining process is described as the process of finding a subset D' of D and hypotheses HU(D',C) about D' that a user U considers useful in an application context C. Note that D' may not only have fewer data elements than D but it may also have a lower dimensionality (m').

The hypotheses expressing interesting aspects of the data may deal with the whole database or with a single relation (D' = D or D' = R_i) they may deal with real subsets of the database ($D' \subset D$ with |D'| << |D| and |D'| sufficiently large) or with single exceptional data items, so-called hot spots ($D' \subset D$ with |D'| =1 or sufficiently small when compared to |D|). Among others, hypotheses properties that hold for all or most $e_i \in$ D', ($D' \subset D$), classifications of D' into classes C_i with different properties P_i [$P_i(e_1) \neq P_j(e_2)$ => $e_1 \in C_i \wedge e_2 C_j \wedge i \neq j$] functional dependencies F or relationships R between two or more dimensions [d_{i1}= $F(d_{i2}, .., d_{i1})$ or $R(d_{i1}, d_{i1})$, $l \leq m$].

Clustering is a data mining technique used to place data elements into related groups without prior knowledge of the group definitions. It is the process of grouping data objects into a set of disjoint classes called clusters, so that objects within a class have high similarity to each other while objects in separate classes are more dissimilar. Consider a dataset X consisting of data points x_i ($1 \leq i \leq N$) (objects, instances, cases, patterns) where x_i = {a_{i1}, a_{i2}, a_{i3}.....a_{id}} and $a_{ij} \in$ A is

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a numerical or nominal attribute from the attribute space A. It refers to a procedure that assigns data objects to a set of classes. Unsupervised means clustering does not depend on predefined classes while classifying the data objects.

DNA Nanotechnology

DNA nanotechnology is the design and manufacture of artificial nucleic acid structures for technological uses. In this field, nucleic acids are used as non-biological engineering materials for nanotechnology rather than as the carriers of genetic information in living cells. Researchers in the field have created static structures such as two- and three-dimensional crystal lattices, nanotubes, polyhedra, and arbitrary shapes, as well as functional devices such as molecular machines and DNA computers. The field is beginning to be used as a tool to solve basic science problems in structural biology and biophysics, including applications in crystallography and spectroscopy for protein structure determination. Potential applications in molecular scale electronics and nanomedicine are also being investigated.

Molecular Docking

In the field of molecular modelling, molecular docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Knowledge of the preferred orientation is used to predict the strength of association or binding affinity between two molecules using scoring functions. The associations between biologically relevant molecules such as proteins, nucleic acids, carbohydrates, and lipids play a central role in signal transduction. The relative orientation of the two interacting partners affect the type of signal produced. Docking is frequently used to predict the binding orientation of small molecule drug candidates to their protein targets and predict the affinity and activity of the small molecule. Hence docking plays an important role in the rational design of drugs [1]. The aim of molecular docking is to achieve an optimized conformation for both the protein and ligand and relative orientation between protein and ligand such that the free energy of the overall system is minimized.

Molecular docking is a problem of "lock-and-key", where one is interested in finding the correct relative orientation of the "key" which will open up the "lock". The protein can be thought of as the "lock" and the ligand can be thought of as a "key". Molecular docking is defined as an optimization problem, which would describe the "best-fit" orientation of a ligand that binds to a particular protein of interest. Both the ligand and the protein are flexible, a "hand-in-glove" analogy is more appropriate than "lock-and-key". The ligand and the protein adjust their conformation to achieve an overall "best-fit" and conformational adjustments resulting in the overall binding is referred to as "induced-fit" [2]. There are two key parts to any docking program, namely a search of the configurational and conformational degrees of freedom and the scoring or evaluation function. The search algorithm must search the potential energy landscape in enough detail to find the global energy minimum. In rigid docking the algorithm explores different positions for the ligand in the receptor active site using the translational and rotational degrees of freedom. Flexible ligand docking adds exploration of torsional degrees of freedom of the ligand to this process.

II. RELATED WORK

DNA nanotechnology focuses on creating nucleic acid systems with designed dynamic functionalities related to their overall structures, such as computation and mechanical motion. There is some overlap between structural and dynamic DNA nanotechnology, as structures can be formed through annealing and then reconfigured dynamically, or can be made to form dynamically in the first place[3][4].

- **Structural design**

  The first step in designing a nucleic acid nanostructure is to decide how a given structure should be represented by a specific arrangement of nucleic acid strands. This design step determines the secondary structure, or the positions of the base pairs that hold the individual strands together in the desired shape. Several approaches have been demonstrated [5].

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- **Tile-based structures.**

  This approach breaks the target structure into smaller units with strong binding between the strands contained in each unit, and weaker interactions between the units. It is often used to make periodic lattices, but can also be used to implement algorithmic self-assembly, making them a platform for DNA computing. This was the dominant design strategy used from the mid-1990s until the mid-2000s, when the DNA origami methodology was developed [6].

- **Folding structures.**

  An alternative to the tile-based approach, folding approaches make the nanostructure from a single long strand. This long strand can either have a designed sequence that folds due to its interactions with itself, or it can be folded into the desired shape by using shorter, "staple" strands. This latter method is called DNA origami, which allows the creation of nanoscale two- and three-dimensional shapes [7].

- **Dynamic assembly.**

  This approach directly controls the kinetics of DNA self-assembly, specifying all of the intermediate steps in the reaction mechanism in addition to the final product. This is done using starting materials which adopt a hairpin structure; these then assemble into the final conformation in a cascade reaction, in a specific order. This approach has the advantage of proceeding isothermally, at a constant temperature. This is in contrast to the thermodynamic approaches, which require a thermal annealing step where a temperature change is required to trigger the assembly and favor proper formation of the desired structure [8].

III. MOLECULAR DOCKING APPROACHES

In Molecular docking three approaches are popular. First approach uses a clustering technique that is applied to reduce the number of potential solutions. Second approach uses a matching technique that describes the protein and the ligand as complementary surfaces. The third approach simulates the actual docking process in which the ligand-protein pair wise interaction energies are calculated.

Clustering techniques for docking

Dima Kozakov, Karl H. Clodfelter, Sandor Vajda, and Carlos J.Camacho have introduced [9] optimal clustering for detecting near-native conformations in protein docking. Two different clustering strategies are developed to predict docked conformations based on the clustering properties of a uniform sampling of low free-energy protein-protein and protein-small molecule complexes. Guillaume Bouvier, Nathalie Evrard-Todeschi, Jean-Pierre Girault and Gildas Bertho have proposed [10] automatic clustering of docking poses in virtual screening process using Self-Organizing Map. A compound clustering is very tedious due to the large number of contacts extracted from the different conformations proposed by docking experiments. F. Roummel Marcia, Hulie have developed [11] global optimization in protein docking using clustering, underestimation and semi definite programming. This work solves the underestimation problem using SDP and present numerical results for active site prediction in protein docking.

Stephan and Yang have proposed [12] identification of near-native structures by clustering protein docking conformations. Protein-Protein docking algorithms use the Fast Fourier Transform technique to sample the six-dimensional translational and rotational space. John Preiestle has introduced [13] 3-D clustering: a tool for high throughput docking. This program clustering docking poses based on their 3- dimensional (3D) coordinates as well as on their chemical structures. W. Tong, Z. Weng have applied [14] clustering Protein-Protein docking predictions. This work describes a clustering algorithm for improving Protein-Protein docking predictions. This algorithm was applied to two sets of predictions for 36 test cases, one set generated with a rigid-body docking algorithm. W. Anisha Goorah, David Ritchee have developed [15] spatial clustering of protein binding sites for template based protein docking. KBDOCK, a 3D database approach for spatially clustering protein binding sites and for performing template-based protein docking. Table 1 shows the clustering techniques for docking.

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Shape Complementarity Approach

Several methods are available in the survey to perform Flexible Protein-Ligand Docking to find the ligand binding site. The methods are Geometric matching, shape complementarity, Graph representation, Shape matching, and Fourier shape descriptor. The complementarity between the two surfaces amounts to the shape matching description that may help finding the complementary pose of docking the target and the ligand molecules. Another approach is to describe the hydrophobic features of the protein using turns in the main-chain atoms. One more approach is to use a Fourier shape descriptor technique. Whereas the shape complementarity based approaches are typically fast and robust, they cannot usually model the movements or dynamic changes in the ligand/ protein conformations accurately, although recent developments allow these methods to investigate ligand flexibility. They are also much more amenable to pharmacophore based approaches, since they use geometric descriptions of the ligands to find optimal binding.

S. Bashir and Z. Zsoldos have demonstrated [16] that Geometric methods can be used to solve Protein-Drug Docking problem and analyse the search problem from a computational perspective. RigiDock algorithm, Pose Match algorithm and polynomial time algorithm are used to solve the closed predicted pose to the native structure. A polynomial time algorithm is developed for the matching phase of the docked rigid fragments. Certain scoring function conditions are used to find the optimality of the proposed algorithm. Chandrajit Bajaj, Rezaul Chowdhury and Vinay Siddavanahalli have addressed [17] this problem by adapting Fast Fourier approach. This work is extended from non uniform Fast Fourier Transform-based docking algorithm to include an adaptive search phase. F^2 Dock is based on an extensive experimental study on a list of benchmark complexes and solutions based on desolvation energy. Apostolos Axenopoulos, Petros Daras, Georgios Papadopoulos and N. Elias Houstis have presented [18] a shape descriptor for fast complementarity matching in Molecular docking based on Geometric complementarity. A set of local surface patches is generated based on the local surface. The result proves that the shape complementarity method demonstrates superior performance over other well-known geometry based rigid-docking approaches.

Tao Zhang *et.al*, have applied [19] graph based approach for protein-protein docking. Protein-Protein Docking is the computational approach to predict protein-protein interactions, and the results demonstrate the reliability of this approach. A.Luis Diago and Ernesto Moreno have proposed [20] an evaluation of between molecular surfaces using compactly supported radial basis functions. The scoring of energetic function is the one that must fulfil this function. The compactly supported radial basis function is proposed to create analytical representations of molecular surfaces, which are then included as key components of a new scoring function for molecular docking. Peggy Yao *et.al*, have developed [21] an efficient algorithms to explore conformation spaces of flexible protein loops. The seed sampling algorithm samples broadly from this space while the deformation sampling algorithm uses seed conformations as starting points to explore the conformation space around them at a finer grain.

Table 1. Clustering techniques for docking

Author, Year	Paper Title	Algorithm(s)	Features
Dima Kozakov, Sandor Vajda, and Carlos J. Camacho, 2005	Optimal clustering for detecting near-native conformation in protein docking	Optimal Clustering	Used for ranking and discrimination of protein-protein complex structures. Clusters the 4N receptor-ligand filtered structures according to the root-mean-squared deviations.
Jean-Pierre Girault and Gildas Bertho, 2009	Automatic clustering of docking poses in virtual screening process using Self-Organizing Map.	Self Organising Map	To discriminate active compounds from inactive ones with careful analysis of inter atomic contacts between the molecule and the target.
F. Roummel Marcia, Hulie, 2007	Global optimization in protein docking using clustering	Docking Mesh Evaluator Algorithm	The underestimation of data points by a convex quadratic function is a useful tool for approximating the location of the global minima of potential energy functions that arise in protein-ligand

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			docking.
W Tong, Z Weng, 2004	Clustering protein-protein docking predictions	ZDOCK Clustering	Applied to two sets of predictions for 36 test cases, one set generated with a rigid-body docking algorithm ZDOCK.
W. Anisha Goorah, David Ritchee , 2007	Spatial Clustering of protein binding sites for template based protein docking	Spatial Clustering algorithm	KBDOCK combines residue contact information from the 3DID database with the Pfam protein domain family classification together with coordinate data from the PDB.

Kahraman, R.J Morris and R.A Laskowski have presented [22] a shape variation in protein binding pockets and their ligands. The normalisation procedure of the standard spherical harmonic coefficients enabled the investigation of the contribution of shape and size to the classification performance. Shape alone outperforms the contribution of size alone in the classification, but size does surprisingly well clefts to clefts and ligands to ligands. T.R Alasdair Laurie and M.Jackson have proposed [23] the method for the prediction of Protein-Ligand Binding sites for structure based drug design and virtual ligand screening. Structure based drug design is a computational approach to lead discovery that uses the three dimensional structure of a protein to fit drug like molecules into a ligand binding site to modulate function. Binding site prediction has been used in several projects and has been incorporated into several docking tools. Geometric shape complementarity methods describe the protein and ligand as a set of features that make them dockable [24]. These features include molecular surface or complementary surface descriptors. The receptor's molecular surface is described in terms of its solvent accessible surface area and the ligand's molecular surface is described in terms of its matching surface description.

III.SIMULATION TECHNIQUE

The simulation of the docking process as such is a much more complicated process. In this approach, the protein and the ligand are separated by some physical distance, and the ligand finds its position into the protein's active site after a certain number of "moves" in its conformational space. The moves incorporate rigid body transformations such as translations and rotations, as well as internal changes to the ligand's structure including torsion angle rotations. Each of these moves in the conformation space of the ligand induces a total energetic cost of the system, and hence after every move the total energy of the system is calculated. Table 3 shows the simulation techniques used in docking.

E. Kiruba Nesamalar and C.P Chandran have developed [25] HClustSwarmDock: a web server for flexible protein-ligand docking using hierarchical clustering with Swarm Intelligence. A New algorithm HClustSwarmDock is proposed which is based on the PSO combined with Hierarchical Clustering technique. PSO is a computational method that optimizes a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. The search capacity and the docking accurateness of HClustSwarmDock are evaluated by multiple docking tests.

E.Kiruba Nesamalar and C.P Chandran have proposed [26] a Web-Enabled system design for molecular docking. This work presents "KNC-Dock", and it is based on the SwissDock engine, combined with setup scripts for curating common problems and for preparing both the target protein and the ligand input files. Monte Carlo algorithms, "Lamarckian" GA, and Granular Computing are implemented in KNC-Dock. An Efficient AJAX/PHP interface was designed and implemented the submit dockings and retrieve the predicted complexes. The web server also provides an access to a database of manually curated complexes [27].

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Table 3. Simulation techniques used in docking

Author, Year	Tool Name	Algorithm(s)	Features	Tool Link
E.Kiruba Nesamalar, C.P. Chandran, 2012	HClustSwarmDock	Hierarchical clustering with PSO	HClustSwarmDock is shown by computer simulation and it performs well in obtaining accurate conformations lesser binding energy and robustness.	http://hclustswarmdock.com
E.Kiruba Nesamalar, C.P. Chandran, 2011	KNC-Dock	Genetic Algorithm	"KNC-Dock", a web server dedicated to the docking of small molecules on target proteins. It is based on the SwissDock engine.	http://kncdock.scripps.edu
Aurelien Grosdidier, Vincent Zoete Olivier Michielin, 2011	SwissDock	EADock ESS Algorithm	SwissDock: a web server dedicated to the docking of small molecules on target proteins. It is based on the EADock DSS engine.	http://swissdock.vital-it.ch/docking
Xiyuan Hou, Olga Sourina, 2010	HMolDock	Haptic Rendering Algorithm	HMolDock: Haptic devices enable the user to manipulate the molecules and feel interactions during the docking process in virtual environment on the computer.	http://hmoldock.com
Imre Pechan, Bela Feher, Attila Berces, 2010	AutoDock	Lamarckian Genetic Algorithm	AutoDock: is popular software for the bioinformatics related molecular docking problem. The FGPA based acceleration of AuoDock is used.	http://autodock.scripps.edu
Nicolas Ferey, Guillaume Bouyer, Christine martin, 2008	HOSMOS Dock	Hierarchical task analysis algorithm	Protein-Protein docking is a recent practice in biological research which involves using 3D models of proteins to predict the structure of complexes formed by these proteins.	http://hosmos.scripps.edu
Yong Zhao, F. Michel Sanner, 2007	FlipDock	Genetic Algorithm	Conformational changes of biological macromolecules when binding with ligands have long been observed and remain a challenge for automated docking methods.	http://flipdock.scripps.edu
Ting-Cheng Lu, JinHui Ding, N.Silvia Crivelli, 2005	DockingShop	Conformational Search space algorithm	DockingShop is an intergrated environment for interactively steering molecular docking by navigating a ligand or protein to the receptor's estimated binding site.	http://dockingshop.scrips.edu

Xiyuan Hou, Olga Sourina have proposed [28] a haptic rendering algorithm for biomolecular docking with torque force. Implementation of torque feedback allows the user to have more realistic experience during force

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simulation and find the optimum docking positions faster. It enables the user to experience six degree-of-freedom (DOF) haptic manipulation in docking processes. The linear smoothing method was proposed to improve stability of the haptic rendering during molecular docking.

IV. MOLECULAR DOCKING OPTIMIZATION ALGORITHMS

E.Kiruba Nesamalar and C.P Chandran have developed [29] Fuzzy Clustering with ACO for Protein-Ligand Docking. A new algorithm called Fuzzy clustering Ant Colony Optimization is proposed for solving Molecular Docking problems. E. Kiruba Nesamalar and C.P Chandran have presented [30] Genetic clustering with BCO for flexible Protein-Ligand docking. E.Kiruba Nesamalar and C.P Chandran have proposed [31] Integration of Data Mining concepts with Granular Computing for Molecular Docking and mainly applied to structure-based drug design. The molecule docking problem is to predict the three dimensional structure and the affinity of a binding of a target receptor and a ligand. Mohamed Wahib, Asim Munawar, Masaharu Munetomo and Kiyoshi Akama have demonstrated a Bayesian optimization algorithm for de novo ligand design based docking running over (Graphical Processing Unit) GPU. It introduces the use of GPU to overcome the very long time required in evaluating each possible fragment combination.

Yu Liu, Wentao Li, Yongliang Wang, and Mingwei lv have presented based on a variant of PSO named Fully Informed Particle Swarm and the semi empirical free energy force field in AutoDock 4.0, a new approach to flexible docking method called FIPSDock was implemented.

V. CONCLUSION

This survey focused on clustering techniques and optimization algorithms. Three approaches have been discussed in this literature. One approach uses a matching technique that describes the protein and the ligand as complementary surfaces. The second approach simulates the actual docking process in which the ligand-protein pair wise interaction energies are calculated. Three approaches have significant advantages as well as some limitations. The differences in and performance of available docking software are also discussed. ACO, PSO and BCO algorithms are analysed. In this work it is identified that BCO algorithm has the advantages of strong robustness, fast convergence and high flexibility, and fewer control parameters. Finally it is concluded that BCO algorithm is better to find the positions of interacting ligand and a protein with a minimal energy.

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E.Kiruba Nesamalar was born in Sivakasi, Tamil Nadu (TN), India, in 1988. She received the Bachelor of Computer Science (B.Sc.) degree from the Standard Fireworks Rajaratnam College for Women, Sivakasi, TN, India, in 2008 and the Master of Computer Science (M.Sc.) degree from the Ayya Nadar Janaki Ammal College (ANJAC), in 2010 and Master of Philosophy (M.Phil.) of Computer Science degree from the ANJAC, Sivakasi, TN, India, in 2012 and pursuing her Ph.D in Bharathiyar University, Coimbatore and now she working as an Assistant Professor in the Department of IT, Sri kaliswari College, Sivaksai. Her research interests include data mining, and bioinformatics. She has published 10 research papers in national and international conference proceedings.