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Classification and Prediction ofDrug through Chemical Properties

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ABSTRACT

Rapid growth of drug is increases in our daily life, so drug discovery is very important subject which is used to predict the unknown types of drugs. Drug or medicines is chemical molecules that interact the chemical drug and drug target. Prediction technique is used drug discovery pipeline form target identification of drug target. The drug or medicine is classified physical and chemical properties of their characteristics which include chemical structure, molecular mass and surface area and other chemical properties. Classification and prediction of drug we used optimization technique according to their properties which predict unknown type of drug, it will classify drug of different categorize of drug class. We proposed the weight optimization technique and k nearest neighbor technique to classified and predict unknown type of drug.

Keywords:*prediction of drug, optimization technique, k nearest neighbor.*

I.INTRODUCTION

Research and development drug Pharmacodia is a big platform that obtain detain information of medicines. While entering drug in market they will approved from the state food and drug administration. Multinational industries developing of new drug cost is high due to profitable to compare other drug or medicines. Reducing the drug cost as to the large multinational companies classified a drug is important that specify the content of a drug which calculate similarity between other medicines.

The drug molecules similarity searching is identify unknown type of drug in datasets. We used optimization technique are predict drug molecule thorough their properties and characteristics. Classification of drug or medicine we used simplest k nearest neighbor method are classified drug class, it will identify the different type of categories or class. The drug diseases classification will identify the drug molecules, physical and chemical structure, medicine properties and their characteristics. The drug information includes drug name, indication, molecular structure and chemical properties.

II.RELATED WORK:

In a prediction of drug on the basis of their chemical structure are analyzed and designing drug which are defined to ligand based drug and structural based design,Ligand based approach based on chemical similarity searching using fingerprint method and the structure based method to fragment based design to identify drug target.

The drug chemical genomic identified new drug leads which are interacting with small molecules and drug target molecules [1].The virtual screening is used in drug discovery; they are mostly used in chemical similarity searching based on chemical structure and properties [2]. The structure of molecule has specification of descriptor will compared to other descriptor; it will measure similarity between drugs [3]. Pharmacologicaland genomic spaces can be used to develop computational frameworksfor drug target identification[4].

III.PROPOSED SYSTEM:

In a proposed system classification and prediction of chemical drug we used optimization technique to optimize through weight molecules and classification of drug used k nearest neighbor method to classify unknown type of drug.

A. Optimization Technique:

In drug dataset optimization technique is used to find the optimal solution, the chemical drug has different properties and characteristics of drug. The drug includes information of drug name, chemical structure, indication and molecular structure. The drug physical and chemical properties of drugs includes molecular mass, hydrogen bond donor, hydrogen bond acceptor, flexible rotation keys, polar surface area and hydrophobic constant. Based on these properties we optimize the weight of chemical drug.

- ***Gradient descent algorithm:***

Gradient descent algorithm is an optimization algorithm used to find value of parameter as function that minimized cost function. It must be search for optimization algorithm in chemical drug. The step of gradient descent algorithm as follows.

Step 1: initialize the weights variable with random values and calculate the prediction error.

Step 2: calculate the gradient weight of small value from their original value and calculate their errors w.r.t the weight.

Step 3: adjust the weigh gradient to reach the optimal value and calculate the new prediction errors.

Step 4: repeat the step 3 and step 4 till further adjustment to weight variable significantly to reduce the errors.

B. Classification Baseline:

Classification of chemical drug based on these properties we used the simplest k nearest algorithm to classify a chemical drug. In k nearest neighbor, Euclidean distance formula to classify the chemical drug and calculate similarity between medicines. We used physical and chemical properties of chemical drug to calculating the similarity between medicines. Based on these properties we are classified unknown type of drug upon chemical datasets. They are calculating the distance of existing drug from the training set. The k is the smallest distance from sample and assigns the category of chemical drug class.

IV.CONCLUSION

Classification and prediction of chemical drug we proposed the optimization technique to find the optimal value. The chemical drugs aredefining the properties basis which optimizes the drug or medicines. Predicting drug or medicine we used the gradient descent formula to optimize the chemical drug, it will find the optimal solution of drug. Classification of chemical drug we used k nearest neighbor technique to classify unknown type of drug, they are categories the different type of chemical drug class. We are classify various type of drug based on physical and chemical properties.

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