Department of Artificial Intelligence

22AIE212:Design and Analysis of Algorithms

EPITOPE PREDICTION FOR VACCINE DEVELOPMENT

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CERTIFICATE

This is to certify that this project entitled, "**EPITOPE PREDICTION FOR VACCINE DEVELOPMENT**" submitted by Vada Gouri Hansika ,Malavika S prasad, Katikala Dedeepya and Geshna B is an authentic work carried out by the team under my supervision and guidance. To the best of my knowledge, the content presented in this report has not been previously submitted to any other academic institution, nor has it been utilized to fulfill any degree or diploma.

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1. Introduction

The project, which is "**Epitope Prediction for Vaccine Development**", focuses on the computational prediction of epitopes associated with antigens, which play a critical role in immunization. Epitopes are short peptides or regions of a larger protein that bind with the receptors of immune cells and trigger the response of immunity through secretion of antibodies. These epitopes can be derived from the surface or internal regions of the pathogens, and understanding which peptides would provoke an immune response will arm us with valuable information about designing successful vaccines.

Predicting accurate epitopes remains one of the most difficult and significant tasks in immunology. Established methods usually imply the use of many laboratory experiments, which may take years and are expensive. This leads to the development and increasing popularity of predictive methods based on ML and DL models as a quick substitute for epitope prediction process from protein sequences. This particular project would use modern machine learning methods for the prediction of **B-cell** epitopes, working on datasets obtained from the **Immune Epitope Database (IEDB)** and **UniProt**, containing extensive annotations of peptide sequences and matched immune responses.

Envisaged thus, this web-based tool will empower researchers to make fast epitope predictions based on their protein sequences-an automation driven by the algorithms including those encompassed under the rubric of **Random Forest, LightGBM, XGBoost, catboost, Gaussian NB, LSTM** and **Neural Networks .** The tool will support numerous input formats and will offer visualization of interpretation against prediction modeling results of epitopes predicted along with their ranks of capacity to induce immune responses.

It would also mean that the prediction process will be advanced with other attributes such as peptide-protein interaction analysis, MHC binding affinity, and epitope localization that make predictions biologically relevant and equally applicable to real-world vaccine development. The integration of deep learning and graph-based models will make the most promising leap forward in improving both the precision and efficiency of deducing epitopes.

2. Abstract:

The **Epitope Prediction for Vaccine Development** project aims to bring down the barrier of identifying potential epitopes with the help of high-throughput computational methods. These epitopes are antigen peptides that can trigger the immune system. Their identification is a critical step in vaccine design, allowing selecting sequences of peptide that would ideally B-

stimulate an immune response. Traditional experimental methods for epitope identification are rather time-consuming and expensive, which is why one has shifted towards machine learning (ML) and deep learning (DL)-based approaches for prediction with better efficiency and accuracy.

The project applies numerous machine-learning algorithms like Random Forest, XGBoost, LightGBM, and CatBoost. In addition, neural networks such as feed-forward neural networks (FNN) and long short-term memory networks (LSTM) are utilized for predicting epitopes from the protein sequences. The model primarily predicts B-cell epitopes using datasets from the Immune Epitope Database (IEDB) and UniProt. Important prediction indicators include peptide-protein interaction, MHC binding affinity, and epitope localization.

The final output of this project is the development of a web-based tool where the user can upload test csv file, make predictions, and visualize results. The tool also ranks epitopes based on biological relevance for vaccine design. Hence, the present study provides a scalable, fast, and usefully reliable option to epitope prediction by combining these computational models, with vast applications for vaccine research and immunotherapy.

3. Objectives

1. **To Develop a B-cell Epitope Prediction Model:**
   The ultimate goal is to develop a robust machine learning and deep learning-based model in predicting B-cell epitopes. This would primarily focus on the identification of peptides capable of binding to **B-cell receptors** and eliciting an immune response, therefore being essential in designing vaccines and immunotherapies.
2. **To Use the Existing Databases to Create Dataset:**
   - The project will utilize curated datasets from the **Immune Epitope Database (IEDB)** that provide in-depth details about protein sequences and their corresponding epitopes. These datasets will be the basis for training the model so that the predictions made are relevant and accurate.
3. **To Implement Several Prediction Algorithms and Compare Them:**
   - A number of machine learning (ML) models such as Random Forest, XGBoost, LightGBM, Gaussian NB and CatBoost will be trained and tested for the purpose of B-cell epitope prediction. Besides, deep learning-based models such as Feedforward Neural Networks (FNN) and LSTM will be investigated for the improvement of prediction accuracy.

4. **To Extract Key Features for Prediction:**
    - Relevant features from **protein** and **peptide** sequences, including **hydrophobicity, aromaticity, stability,** and **relative surface accessibility**, will be extracted and incorporated into the model enhancement. The importance of these features will be elaborated in the context of the immunogenicity of the epitopes.
5. **To Rank Epitopes Based on Immunological Relevance:**
    - After prediction of B-cell epitopes, ranking will be done on the basis of biological scores such as **antigenicity** and **hydrophobicity,** with a greater weight assigned to the more relevant parameter in each case through a composite scoring system. This ranking will allow the selection of the most promising epitopes for experimental validation.
6. **To Develop a User-Friendly Web Interface:**
    - A web-based tool will be developed in order to facilitate the uploading of protein sequences by the user, selection of predictive models, and visualization of results. Detailed predictions will be made along with the ranking of B-cell epitopes, thus providing a solution that is practical and accessible to users for epitope prediction.
7. **To Validate the Predictions with Experimental Data:**
    - Even though the focus of the project is on computational predictions, wherever experimental data are available, the generated results will be validated against the data to ensure the confidence and practical applicability of the prediction models in real vaccine development.

4. System Architecture:

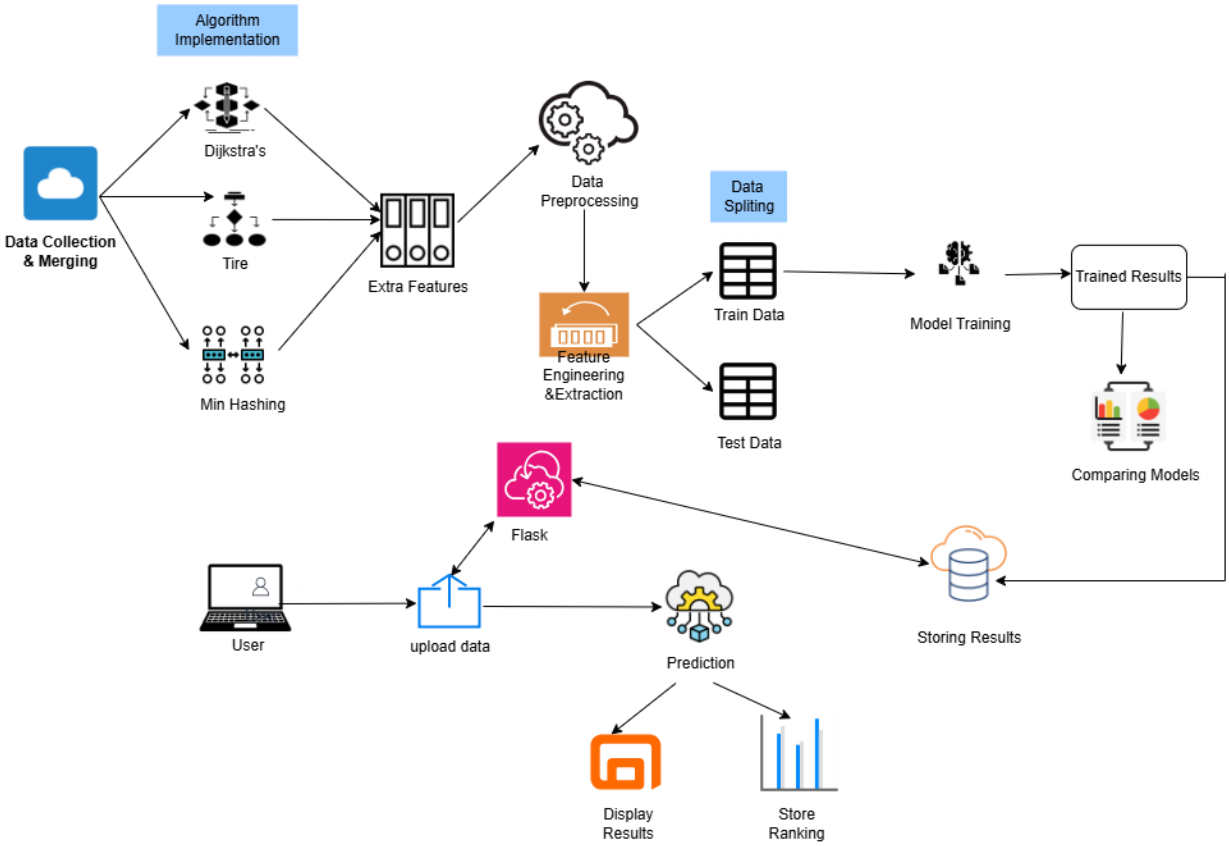

Fig:1

5. Methodology

5.1. Data Collection and Merging:

This project begins with the collecting of two main datasets:

input_bcell.csv: Consists of labeled data for B-cell epitopes, including protein and peptide sequences.

input_sars.csv: Another dataset consisting of peptide sequences from SARS-related proteins added to the initial set so as to increase diversity within the data for better model performance.

After these two datasets are merged together, they yield a comprehensive dataset consisting of peptide and protein sequences together with their respective epitope labels. This is used as the basis for feature extraction and model training.

5.2. Data Preprocessing:

The merged dataset undergoes preprocessing prior to the needed analyses:

Cleansing of Missing Data: Missing values are handled either by imputing a value for them or by omitting those rows that are significantly lacking in data.

Encoding: Proteins and peptides sequences are converted into numerical values (such as by way of one-hot encoding or through embeddings) to allow them to enter into the machine learning models.

Normalization: Continuous features are scaled (such as hydrophobicity, stability, aromaticity, downstream peptide-related features) for standardization.

5.3. Algorithms Application:

In the next step, application of DSA would extract meaningful features that would strengthen the prediction capability of the model. The following algorithms are thus enlisted:

5.3.1 Dijkstra's Algorithm: Used for optimizing graphical data structures that would trace a shorter path between biological interactions or sequence similarity pertaining to the peptides and protein sequences. This would add these new features to the dataset for better comprehension into the relationship among sequences.

5.3.2 Min Hashing: This comes under locality-sensitive hashing (LSH) and is used to downsize a huge peptide sequence dataset. In simple terms, applying Min Hashing implies creating compact representations for the peptides and adding the hashes as features to the dataset, thereby helping the model address large sequence datasets.

5.3.3 Trie Data Structure: While managing an enormous multidimensional dataset, Trie (prefix tree) decreases the indexing time of peptides by enabling quick string matching on them. Trie features such as sequence length, common prefixes, and structural similarities are extracted and appended to the dataset. It comprises good sequence-based features that can provide some insight into the peptide's potential to be an epitope.

5.4. Feature Extraction and Engineering:

In addition, to further the model's prediction ability used in the DSA algorithms, still more features are extracted.

Protein features: Isoelectric point, hydrophobicity, aromaticity, and stability are computed from the protein sequences, which play a key role in determining the overall structure and function of the proteins.

Peptide features: Those properties of peptides called Chou-Fasman (β-turn), Emini

5.5. Model Selection and Training:

A merged and feature-engineered dataset is then used to set up training for several machine learning models that are used to predict B-cell epitopes. Models selected for the training include

5.6 Machine Learning Models:

- **Random Forest (RF):** It is an ensemble model that aggregates the predictions from different decision trees, which makes it suitable for capturing the complex relationships of data.
- **XGBoost:** A gradient boosting algorithm acknowledged for its speed and performance, particularly in the classification task.
- **LightGBM:** A gradient-boosting variant that speeds up training through histogram-based techniques, especially on large datasets.
- **CatBoost:** A solid gradient boosting model that takes care of categorical features. It is good at dealing with the peculiarities of peptide sequence data.

5.7. Deep Learning Model:

- **Feedforward Neural Network (FNN):** This deep learning model captures non-linear data patterns; it serves as a powerful means of classification for complex biological data. The models are being trained under cross-validation conditions to avoid overfitting and guarantee that the results are generalizable.

5.8. Epitope Prediction and Ranking:

Once the models are trained, they classify the peptide sequence in the dataset as a B-cell epitope or non-epitope. This process is carried through the following steps:

Prediction: The peptide sequence is classified using the trained models.

Ranking: Predicted epitopes are ranked according to the probability of being recognized by the immune system. The ranking uses features, such as antigenicity (e.g. Kolaskar-Tongaonkar), hydrophobicity (e.g. Parker), and surface accessibility (e.g. Emini). Thus, higher-ranked epitopes would trigger an immune response.

5.9. Model Evaluation:

The models are assessed based on relevant criteria for classification metrics:

- Accuracy: The fraction of correctly predicted instances with respect to the overall number of instances.
- Precision: This is the proportion of true positive predictions out of the total positive predictions.
- Recall: This is the proportion of true positive predictions out of the positives generated.
- F1-Score: The F1-Score is the harmonic mean of precision and recall, with more importance given to the lower figure.
- ROC-AUC: True positive rate occurred versus false positive rate to give an overall estimate of the model performance in classical functions of imbalanced data.

These are the parameters one can use to appraise the robustness of these models against predicting B-cell epitopes.

5.10. Visualization and Interpretation of Results:

Once the predictions are run, they are visually represented to assist with the interpretation and understanding of the model output:

Tabular Format: The results are presented in a table that identifies the peptide sequences, predicted values (epitope or non-epitope), and available values for corresponding features.

Ranking Plot: The highest 10 ranked epitopes can be presented in a bar plot format, which will provide an overview of which epitopes are most likely to spur an immune response.

5.11. Web Interface:

A web-based interface is developed to allow users to upload their datasets, select models, view predictions, and visualize results. The interface also provides options for downloading the prediction results and ranking plots.

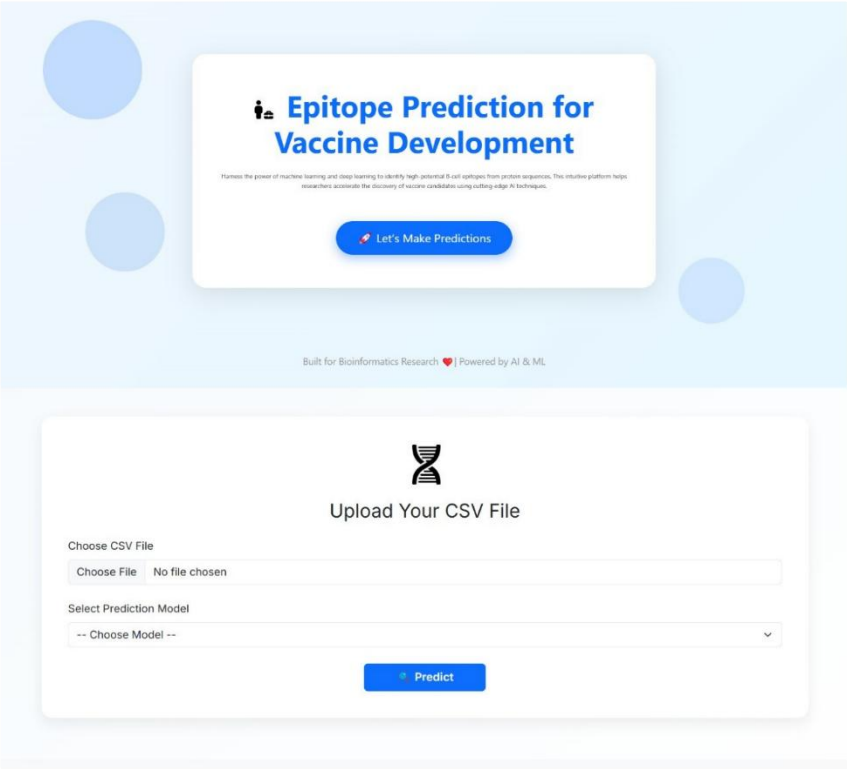

Fig:2 – Web interface

6. Models and Algorithms

6.1.1. Dijkstra's Algorithm:

Dijkstra's Algorithm is one of the famous algorithms that help in finding the most optimal possible route between defined nodes of a graph. In this project, it was applied to represent protein-peptide relationships as graphs, such that the nodes represent peptides or protein sequences, and the edges show how similar they are or how likely they can interact with each other.

Aim:

The main aim is to improve the relationship between peptide and protein sequences according to the evaluation of the shortest route (minimal distance) with respect to similarity or interaction in the sequences.

This can also assess the closeness between different peptides towards a protein, defining the chances for epitopes' classification purposes.

Feature Extraction:

The distances being evaluated using Dijkstra's Algorithm are added as new features to the dataset which will allow the model to include sequence proximity while making predictions.

6.1.2. Min Hashing

Overview:

Min Hashing is a type of local sensitive hashing to enable related processing of high dimensional sets and to find approximate similarities between sets, such as protein and peptide sequences. Here, it becomes useful in cases of computational intensive exact matches while an approximate similarity suffices.

Objective:

The primary goal of Min Hashing in this project is to shrink the size of peptide sequences and at the same time, maintains their similarity.

This technique could make such compact representations (hash signatures) for peptides so that it would be easier for the learning factor to understand and shine pattern recognition among large datasets.

Feature Extraction:

These generated hash signatures from Min Hashing will be the new features added into dataset that cater for peptide similarity in a reduced form.

6.1.3. Trie Data Structures

Overview:

Trie is a tree-like data structure to index strings using nodes to represent each character of a string and edges to represent character transitions. Tries are beneficial for string matching because they support efficient searches with common prefixes, substring matching, and other sequence-related operations.

Purpose:

The investigation of this project needs Tries to index peptide sequences to point out shared prefixes or shape similarities among sequences.

Indexing of the sequences will enable feature extraction pertaining to peptide length, common prefixes, and other structural similarities that determine epitope potential.

Feature Extraction:

Trie-based features such as sequence lengths, prefix occurrences, and common structures extracted and added to the dataset will then allow the machine-learning models to learn better sequence-level patterns which indeed are indicative of epitope characteristics.

6.2.Machine Learning Models

6.2.1. **Random Forest (RF)**

Overview:

Random forest is an ensemble approach to learning based on a decision tree. It creates a multitude of decision trees during training and listens to the mode of the classes for the classification task.

Random forests combine several decision trees constructed from bootstrapped samples of the dataset by taking a majority vote from the predictions given by these trees.

Purpose:

Random forest is used because it is said to generalize well to unseen data and is robust against any overfitting regime in the presence of many features, as is the case with biological datasets like epitope prediction. The method performs very well on high-dimensional data sets and is capable of dealing with numeric and categorical features.

Advantages:

- Deals with high-dimensional data: This serves as a major concern, as the data set is an amalgamation of protein and peptide sequence features.
- **Interpretability:** The feature importance scores allow feeling the contribution of each feature towards the eventual prediction.

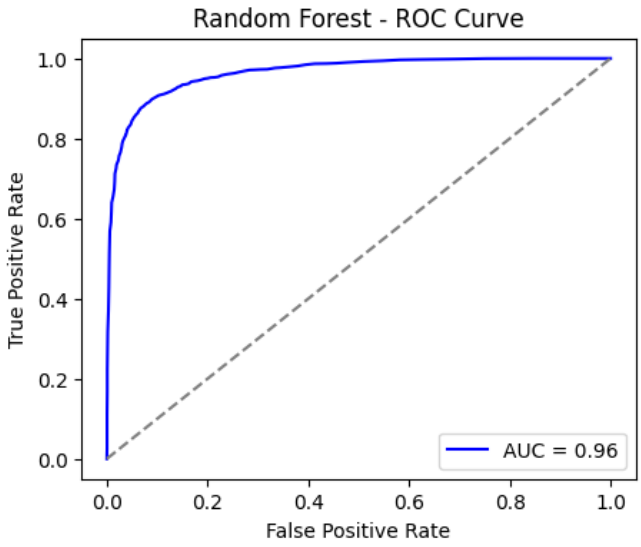

Fig:3

6.2.2 **XGBoost**

Overview:

XGBoost (Extreme Gradient Boosting) is the optimized gradient boosting implementation known to be fast and accurate for classification tasks. New trees are built sequentially, with each new tree being designed to reduce the error of its predecessor on minimizing a loss function.

Purpose:

XGBoost is used because it is computationally efficient for handling large datasets and has had tremendous success in a variety of Kaggle competitions. It is especially useful in handling imbalanced datasets like the epitope prediction problem, where there may be uneven representation of positive and negative classes.

Advantages:

- Efficiency-XGBoost uses advanced optimization techniques that improve the speed and performance of model training (like parallelization and regularization).
- Missing data handling-Does a natural handling of missing values making it quite useful while dealing with biological data that tend to have gaps.
- Accuracy-Reportedly provides a state-of-the-art performance particularly for structured data.

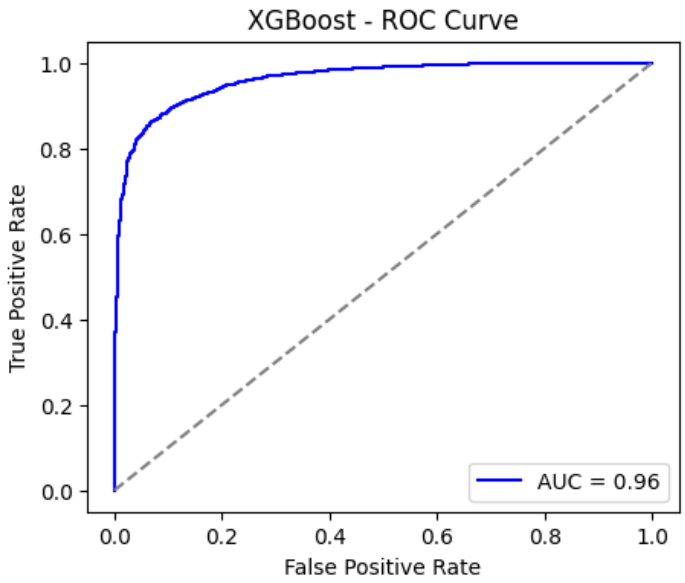

Fig:4

6.2.3 **LightGBM**

Overview:

LightGBM is a kind of boosted gradient tree machine learning algorithm optimized for speed and for large datasets. It does so using histogram algorithms for fast training and low memory consumption.

Purpose:

LightGBM is chosen for being efficient for large datasets and being able to scale. Besides, it can directly handle categorical data without going through preprocessing and is known to outperform XGBoost in many situations.

Advantages:

- Faster Training-LightGBM has a histogram-based method by which it can speed up training, thus suitable for larger datasets from epitope prediction.
- Memory efficient-It avoids a lot of memory operations to give high performance.

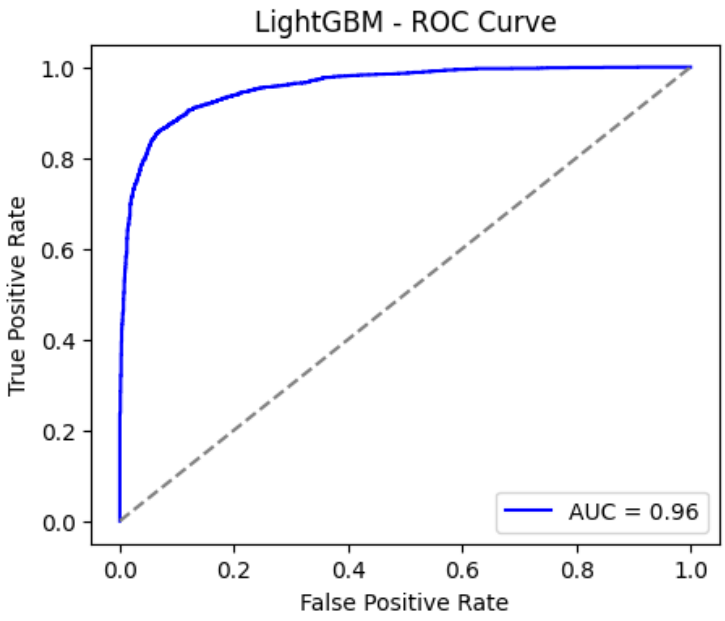

Fig: 5

6.2.4 **CatBoost:**

Overview

Yandex developed the CatBoost software library that provides gradient boosting associated with categorical features. It implements an ordered boosting method for reduced overfitting susceptibility and, therefore, a very stable model yielding satisfactory results with minimal tuning of the parameters.

Applicability:

Due to the presence of categorical data in peptide and protein sequences, which CatBoost can handle naturally, the application of CatBoost is very relevant in this project.

Advantages:

- Automatic Categorical Feature Handling: No need for one-hot encoding or label encoding for categorical features.
- Robustness: CatBoost is robust against overfitting and performs well with less data preprocessing.
- High Accuracy: Often outperforms other models on small to medium-sized datasets, which is the case for B-cell epitope prediction.

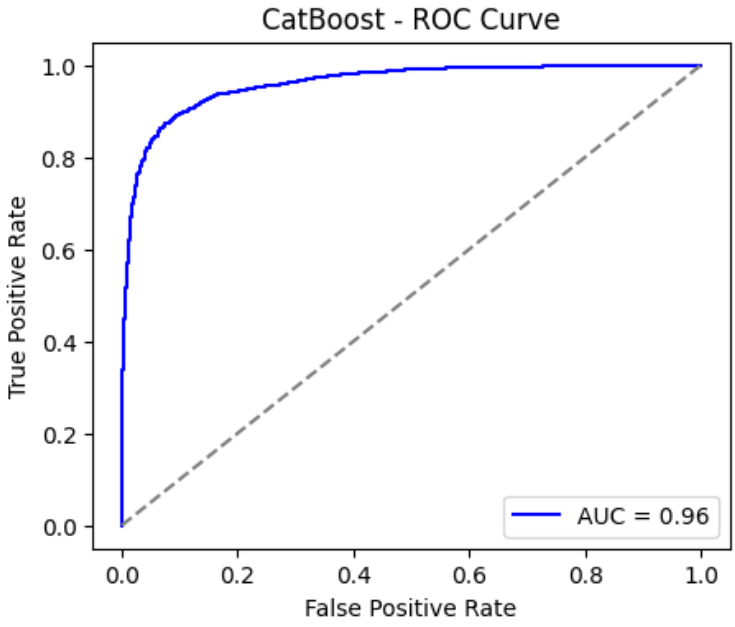

Fig:6

6.2.5 Gaussian Naïve Bayes (GNB)

Gaussian Naïve Bayes (GNB) is a classification algorithm based on Bayes' Theorem, which assumes that all features are independent of each other given the class label. Despite this strong assumption, it often performs surprisingly well in practice, especially in high-dimensional datasets like those used in epitope prediction. The "Gaussian" in GNB refers to the assumption that the continuous features follow a normal (Gaussian) distribution, allowing the model to calculate the likelihood of each feature given a class using the probability density function of a normal distribution.

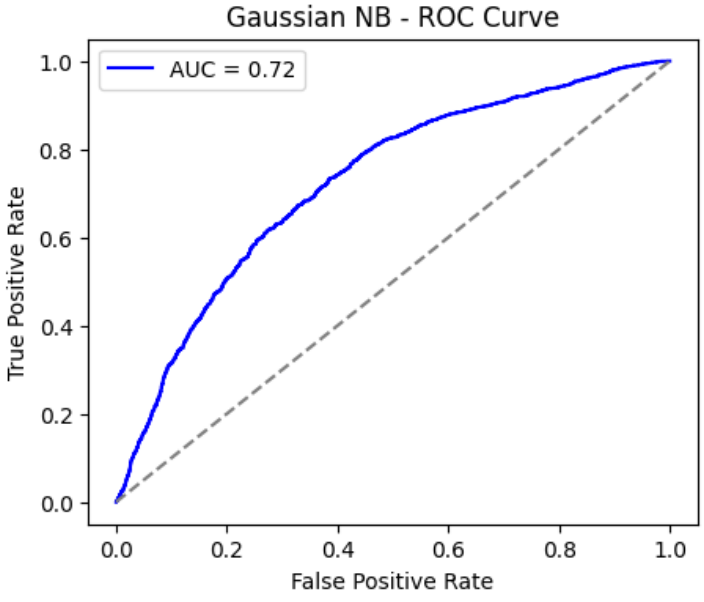

Fig:7

6.2.6 **Feedforward Neural Network (FNN)**

Overview:

A Feedforward Neural Network (FNN) is a deep learning model that consists of several layers of neurons, with the data flowing from input to output in one direction. It is a type of artificial neural network meant to learn non-linear relationships.

Purpose:

FNN captures complex non-linear patterns in the data, particularly with respect to sequence-based features, which may not be fully captured by other machine-learning models.

Advantages:

- Learning Non-linear Patterns: Neural networks are used to model complex relationships between features and outputs, which are very critical in epitope prediction.
- Flexible Architecture: The architecture of the neural network can be varied in accordance with the complexity of the data.

6.2.7. **LSTM (Long Short-Term Memory)**

Overview:

LSTM is a kind of recurrent neural network (RNN) intended to cater for sequential data by memorizing past inputs over lengthy sequences. LSTMs are very convenient in cases where the input data elements are related over a span of many time steps since they can carry meaningful information for a substantial length of time.

Objective:

The use of LSTM in this project is to model the sequential nature of peptide sequences and capture long-range dependencies between amino acid positions, the crux of building spatial and sequential relationship between peptides and their corresponding epitopes.

Advantages:

- Memory retention: LSTMs are meant to remember and learn from long-term dependencies in the data, which helps in the analysis of long sequences like peptides.

- Non-linear pattern recognition: They can recognize complex non-linear relationships between successive data points, which is critical for predicting the immunogenic potential of peptide sequences.
- Handling variations in length inputs: LSTMs are capable of dealing with peptide sequences of varying lengths with no restriction on the length of the input data.

Feature Extraction:

- The LSTM model is trained on peptide sequences, learning the sequential dependencies and encoding this information into its hidden states. The features extracted from the LSTM network's internal states are then added to the dataset, which helps in improving the final prediction accuracy.

7. Dataset Overview

The dataset that has been utilized for the B-cell epitope prediction in this project is taken from different sources. It contains important peptide and protein features that can be used for finding possible epitopes. The primary datasets are:

1. input_bcell.csv: This file is the main training data for B-cell epitope prediction, containing **14,387 rows**. Among these, 14,362 rows correspond to peptide sequences and the 757 remaining rows correspond to proteins. Each peptide sequence has features such as its start and end positions in the protein, peptide sequence itself, and several structural and physicochemical properties characteristics, such as hydrophobicity and stability.

2. input_sars.csv: This file contains some additional training data comprising **520 rows** of peptide sequences regarding the SARS virus. The input attributes have similarities with that of `input_bcell.csv`, which further builds up the training dataset with peptides of importance in pathogens.

3. input_covid.csv: This file consists of the target data for testing; however, no labels are contained in it, making it different from the training datasets. This makes learning from the sequences of peptides associated with COVID-19 exclusive for new epitope predictions.

The dataset is enriched with Chou-Fasman, Emini, Kolaskar-Tongaonkar, and Parker features related to the properties of the peptide sequence that would be beneficial in predicting antigenicity, surface accessibility, and hydrophobicity of peptides. This merged dataset will

be utilized to train the variety of machine learning and deep learning models that will allow accurate and reliable predictions for B-cell epitopes.

8. Exploratory Data Analysis (EDA)

The phase of EDA was characterized by performing several imperative analyses on the combined B-cell epitope dataset in order to comprehend the nature of the data and carefully select appropriate measures for feature engineering and model selection.

- **Feature Distribution:**

The distributions of some important features in the research such as hydrophobicity, stability, aromaticity, and chou_fasman were visualized. Histograms and boxplots were used in this study to examine the dispersion and this uneven distribution.

Nevertheless, the analysis showed that hydrophobicity and stability were normally distributed, whereas much value shown by aromaticity was skewed, so this necessitated transformation.

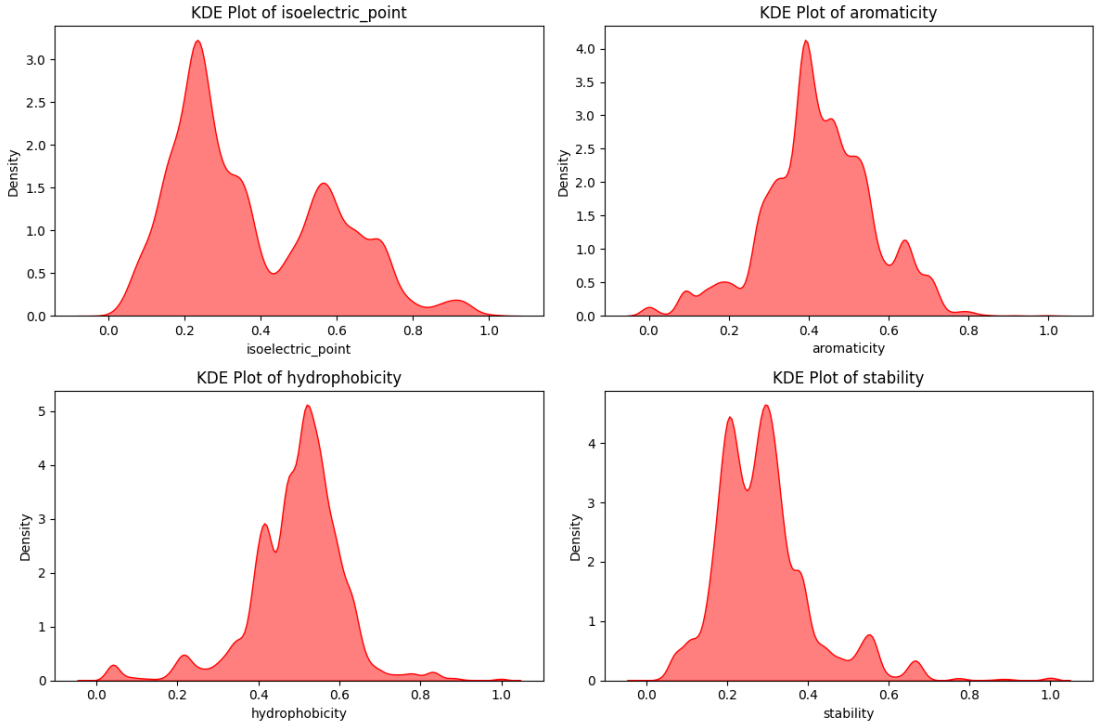

Fig:8 – Feature Class Distribution

- **Correlation Analysis:**

We generated a correlation matrix to establish the relationship existing between the diverse features. This would help us identify highly correlated features (eg. kolaskar_tongaonkar and emini), which would serve as candidates for feature selection regarding multicollinearity handling.

Pearson correlation coefficients were computed to measure linear relationships and help us understand which features can possibly be merged into one or removed to decrease predictive power.

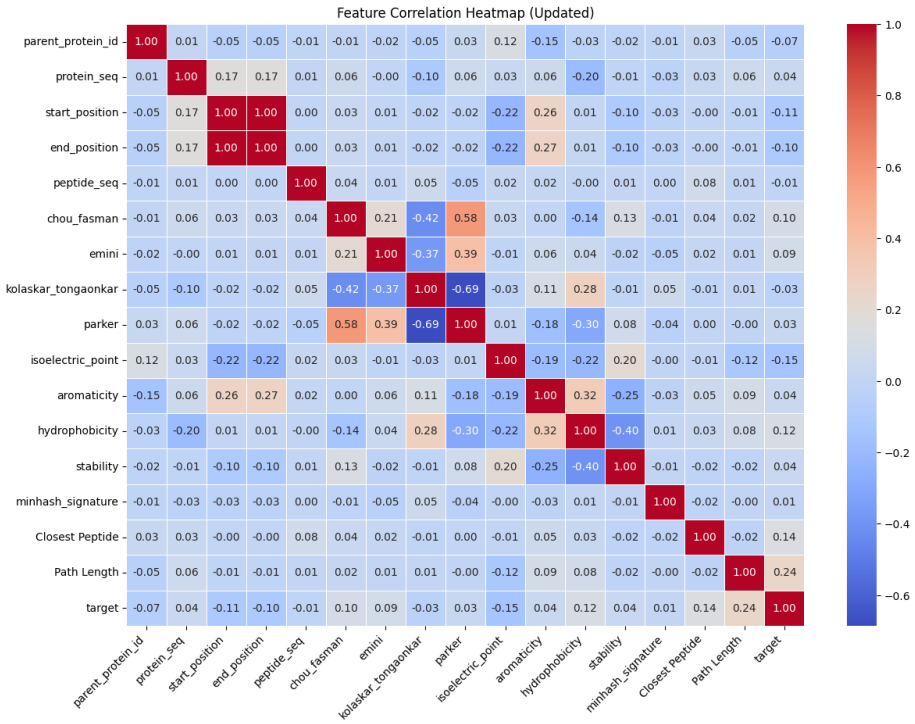

Fig: 9- Correlation

- **Class Distribution:**

The class distribution (epitope vs non-epitope) was visualized in bar charts. We could see that there was an imbalanced dataset in which there were more non-epitope peptides than epitope peptides. This again raised oversampling or altering class weights in the model training to create a balance.

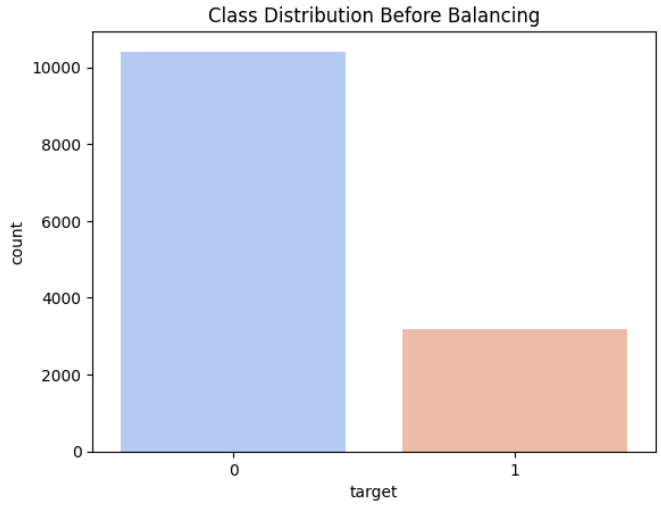

Fig:10 – class Distribution

- **Outlier Detection:**

Numerical features such as isoelectric_point and hydrophobicity detected by box plots were used to display outliers. Winsorization was used in handling outliers as it ensured models were not biased from extremes.

- **Handling class imbalance:**

Because the dataset suffered from class imbalance (more non-epitopes than epitopes), techniques like class weighting and oversampling were utilized to cope with such imbalance during model training. Techniques performed better as models learned to predict pseudoepitopes without bias to the majority class.

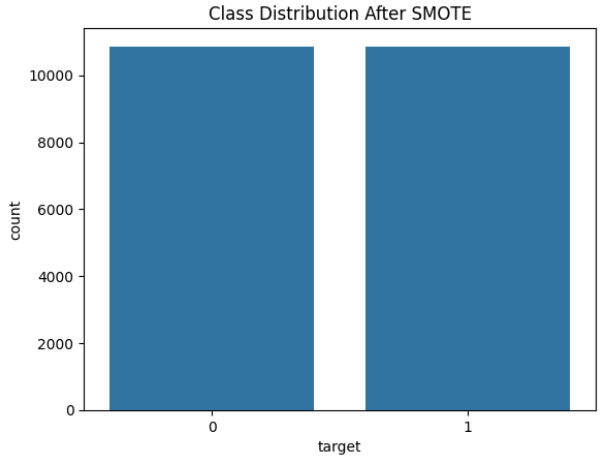

Fig:11

- **Feature Engineering:**

These were normalized from the findings and included features like kolaskar_tongaonkar, emini, and parker to give them an equal weight in the final epitope scoring mechanism.

The insights gained during EDA guided feature engineering and aided in rightly selecting machine learning and deep learning architectures. Discovering patterns essential in the underlying data enabled model optimization for B-cell epitope prediction.

9. Results

The study combined results from machine learning (ML) models and deep learning (DL) models applied to the B-cell epitope prediction task to summarize its key findings. The following paragraph summarises the steps:

Model Evaluation:

It evaluated several models: from conventional machine learning algorithms like Random Forest, Gaussian Naïve Bayes (GNB), XGBoost, LightGBM, and CatBoost to deep learning models such as LSTM and Feedforward Neural Network (FNN).

For all models, metrics such as accuracy, precision, recall, F1-score, and ROC-AUC were assessed. The LSTM and XGBoost models were identified to perform exceptionally well, since they feature in high values of accuracy and F1-score, indicating a favorable capacity for classifying epitopes and non-epitopes correctly with few errors.

The LSTM model was successful at sequentially learning peptide sequences, imparting a very strong prediction basis depending on amino acids.

The importance analysis of features for models such as XGBoost and Random Forest revealed that peptidesequence-related features like kolaskar_tongaonkar and emini were perhaps the most significant for predicting B-cell epitopes.

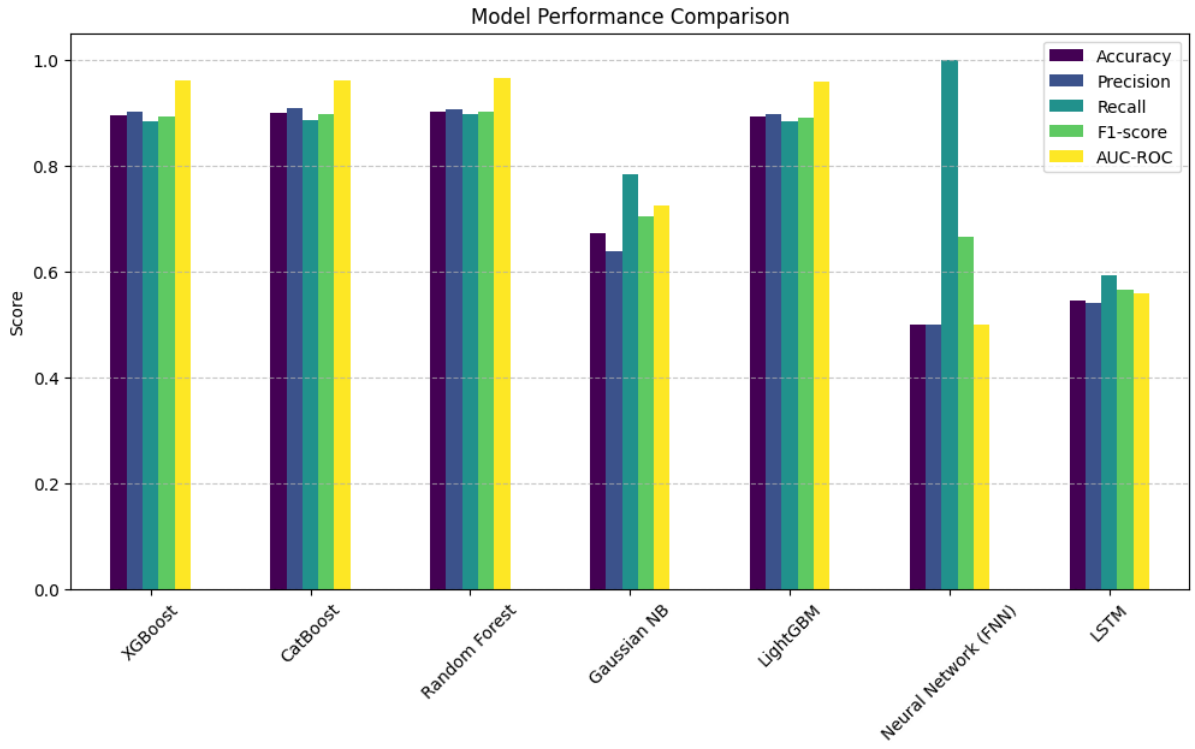

Fig:12 – Models Performance

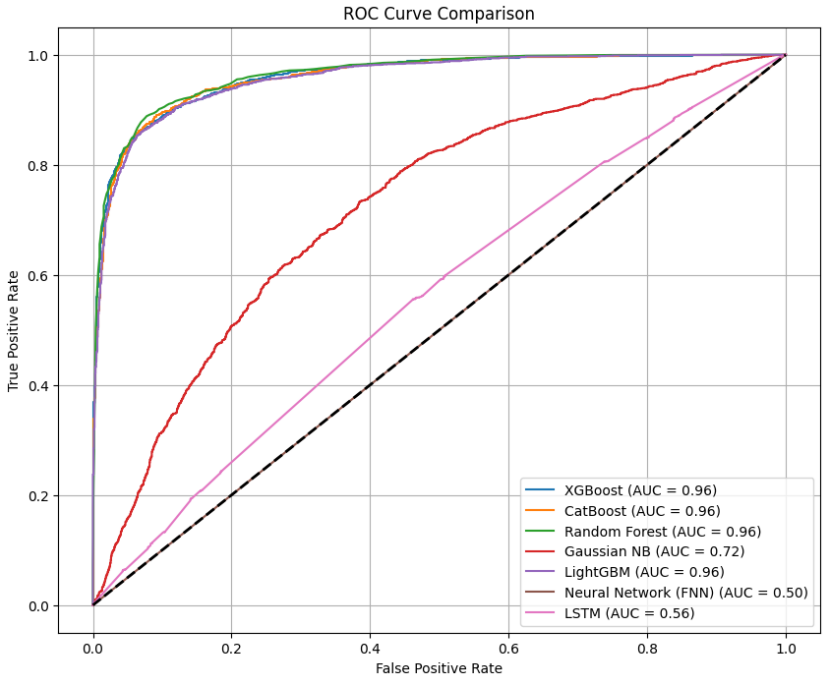

Fig:13- Roc Curve Comparision

10.Emerging Directions for the Future

- **Extension of T-cell Epitope Prediction Modeling:**
  One of the anticipated improvements in this project is the addition of T-cell epitope prediction to make it comprehensive for immune epitope prediction. This could be carried out using either a sequence-based method or a structure-based method for T-cell epitopes.
- **Inclusion of Binding Affinity Data:**
  In addition, future research could feature the incorporation of binding affinity data while predicting T-cell epitopes. In this way, it would move beyond just presence and start predicting affinity for MHC molecules or antibodies, providing a better notion of the immunogenicity of the predicted peptides.
- **Graph Neural Networks (GNN):**
  For instance, GNN integration could suffice in discovering extract relationships that are mathematically complex in peptides and proteins, further increasing prediction accuracy. GNNs have shown promise with the representation of biological sequences as graphs in order to have better extraction features and predictions in bioinformatic workloads.
- **Advanced Features Engineering:**
  Proficient Feature Engineering: Capturing the most minute features from the protein sequences into the models can enhance its performance dramatically by thorough feature engineering, including usage of deep sequence embeddings (e.g., from the models, BERT or ProtBERT) for peptide sequences.
- **Real-time Epitope Prediction:**
  It would also beneficial to set up a real-time epitope prediction system that could score new sequences of epitope from a newly sequenced peptide, particularly in the area of vaccine development. It could be used as an internet-based platform for researchers and health professionals to incorporate in their culturally accepted workflow of vaccine design.
- **Transfer Learning and Model Fine-Tuning:**
  By transferring the learning and fine-tuning of models already learned such as ProtBERT or AlphaFold, more biological knowledge can be levered into the prediction process, especially with regard to their performance over the LSTMs or FNNs from smaller datasets.

- **Extension of DSA Algorithms:**
  Further investigation and optimization of Data Structures and Algorithms (DSA) regarding k-means clustering application or other advanced graph algorithms may show unexplored patterns in peptide-protein interaction-based features for better-designed feature engineering strategies.
- **Model Deployment and User Interface:**
  By building a web-based application, easy access to the B-cell epitope prediction system will be availed. In this way, researchers will easily upload their peptide sequences and receive predictions in real-time with proper ranking and visualization of results.
  This project may hence greatly contribute to vaccine designing and immunotherapy if models continue to be refined and further data appended to the already existing datasets.

11.References

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