*Investigate and Implement KNN Classifier*

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***Abstract—******Algorithms drive the world of machine learning. They’re often praised for their predictive capabilities and spoken of as hard workers that consume huge amounts of data to produce instant results. Among them, there’s an algorithm often labeled as lazy, however it’s quite a performer when it comes to classifying data points - K-Nearest Neighbor (KNN) algorithm.*** ***KNN is a popular supervised machine learning algorithm used for classification and regression tasks. Classification is used to predict the class label of a given input data point, while regression is used to predict the value of a continuous variable for a given input data point. It is also a non-parametric and instance-based algorithm that does not assume any specific probability distribution for data. In KNN, the classification of a new instance is based on the majority class of its k-nearest neighbors in the training dataset. The algorithm relies on finding the k-nearest neighbors of a given data point and assigning a class label based on the majority of those neighbors. In this project, KNN classifier is integrated with Hierarchical temporal memory(HTM) framework to utilize the later for classification task. Specifically, HTM models are capable of learning to represent input data in a feature space with high dimensionality and consequently KNN classifier has been employed to classify the data by considering the closest neighbors within this feature space. This approach is beneficial where the input data exhibits an intricate temporal structure, requiring a more advanced classification approach. KNN model, that is being developed is also integrated with the Neocortex API. The input sequence of data is fed into the encoder and further into the spatial pooler to form a Sparse Distributed Representation(SDR) of the data, which is then being fed into the KNN model for the final classification. Methodologies followed, enhancements performed, and challenges faced are described in detail in subsequent sections of this paper.***

***Keywords— Supervised algorithm; K-Nearest Neighbors; Non-parametric; Hierarchical temporal memory(HTM); Temporal structure; Neocortex API; Sparse Distributed Representation(SDR).***

# **INTRODUCTION**

Machine learning constitutes a pivotal field within computer science, revolutionizing the way computers comprehend and interpret data. The essence of machine learning lies in the development of statistical models and algorithms that can autonomously learn from input data, providing invaluable insights and predictions. One such supervised machine learning algorithm of ML, predominantly used for classification purposes is K-Nearest Neighbors or KNN.

A study, conducted in 2016, in the field of biology and medicine had showed that researchers used KNN classifier to classify patients as either having heart disease or not based on their medical and clinical features. They experimented with the classifier with different values of k to classify the patients and evaluated the performance of the model using metrics such as accuracy, sensitivity, and specificity. The study found that KNN classifier with k=7 achieved an accuracy of 84.5%, sensitivity of 80.6%, and specificity of 88.4%. The model was also able to identify the most important features for heart disease diagnosis, such as chest pain, electrocardiogram results, and age.

Supervised Learning is a machine learning paradigm for acquiring the input-output relationship information of a system based on a given set of paired input-output training samples. As the output is regarded as the label of the input data or the supervision, an input-output training sample is also called labelled training data, or supervised data. The goal of supervised learning is to build an artificial system that can learn the mapping between the input and the output and can predict the output of the system given new inputs. Classification, Regression, Time series prediction, Natural Language Processing (NLP) are some common types of supervised learning algorithm, among others.

Unsupervised learning is a paradigm in machine learning where the algorithm is tasked with exploring and extracting patterns from unlabelled data. Unlike supervised learning, there are no predefined output labels for the algorithm to learn from. Instead, the system aims to identify inherent structures, relationships, or groupings within the data. Reinforcement learning, on the other hand, is a type of machine learning where an agent learns to make decisions by interacting with an environment. The agent receives feedback in the form of rewards or penalties based on the actions it takes, guiding it towards optimal behavior. The goal of reinforcement learning is for the agent to learn a strategy or policy that maximizes its cumulative reward over time.

In this paper, K-Nearest Neighbor (*KNN*) classifier, which comes under the supervised machine learning algorithm is implemented. The KNN model is being developed primarily, which is afterwards incorporated into the Neocortex API. The Neocortex API, in this project, is utilized in order to integrate HTM cortical Learning Algorithm. HTM models, tailored for learning and recognizing patterns in different time-varying data such as sensor data, audio, and video, serve as the input for the KNN classifier. This collaborative utilization between HTM and KNN holds specific significance in scenarios where input data exhibits intricate temporal structures, demanding a more sophisticated classification approach beyond conventional threshold-based methods.

# **METHODS**

This particular section of the paper deals majorly with the following things – a thorough literature review, a detailed theoretical background of KNN, it’s fundamental concept as well as design parameters and HTM. As part of our project, detailed research on KNN and its fundamentals has been conducted, establishing a vivid understanding of the working principle of the implemented supervised machine learning algorithm. In addition to it, HTM has been studied in order to have a clear idea of its functionality, resulting in effective collaboration of the same with the developed KNN model.

## Literature Review

Comprehensive research on KNN has been conducted from the viewpoint of different authors, researchers, and engineers to establish a solid foundation about KNN. This thorough research ultimately helps in designing procedure of the KNN model in the development.

The main objective of the experiment conducted is to utilize the k-Nearest Neighbors (kNN) classifier to categorize unlabeled observations, specifically determining the classification of a sweet potato based on its characteristics. The experiment involves collecting data on crunchiness and sweetness for various labeled examples, such as fruits, vegetables, and grains, and using this information to train the kNN model. By selecting the four nearest labeled examples (apple, green bean, lettuce, and corn) based on the given characteristics, the sweet potato is then assigned to the class with the majority of votes, demonstrating the practical application of the kNN algorithm in classification tasks. It is also noted that average accuracy is the most widely used statistic to reflect the performance of the algorithm. Factors such as k value, distance calculation and choice of appropriate predictors all have significant impact on the model performance[1].

In the study[2] carried out, classification accuracy (CA) and reduction rate (RR) metrics were employed, where CA represents the average classification accuracy for k values of 1, 3, and 5 in the k-Nearest Neighbors (kNN) model. The experimental outcomes reveal that the proposed kNN model method consistently outperforms C5.0 in 5-fold cross-validation and demonstrates comparable performance to traditional kNN. Notably, the kNN model exhibits a significant enhancement in efficiency by preserving only a limited number of representatives for classification purposes. The results illustrate an average reduction rate of 90.41%. At the end, superior classification accuracy and notable efficiency improvements were achieved through the application of the kNN model method across multiple datasets.

The paper[3] focuses on simplifying the understanding of supervised learning and the KNN classification algorithm through easy examples, emphasizing that supervised learning operates on labelled data. The algorithm is demonstrated using a small student dataset, illustrating its application in predicting the pass or fail outcome for a new student based on marks, with a K size of 3 for easy comprehension.

KNN stands out for its computational intensity, requiring more time compared to other algorithms like Neural Networks, which demand extensive training data for precision. The choice between KNN and SVM depends on the size relationship between training data and features, with KNN favoured when data is larger and SVM when features are more numerous. KNN supports non-linear solutions, in contrast to logistic regression, which only handles linear solutions and is relatively faster. Despite its simplicity, KNN lacks efficiency in complex tasks, as it operates without training, making it faster but requiring proper scaling and not always suitable for solutions demanding more sophisticated models [4].

In a nutshell, the conducted literature review suggests some useful insights into KNN. The main advantages of KNN classifier lies with its adaptability to complex datasets, improved efficiency while maintaining optimum computational resources and simplicity. Although computational intensity is one unfriendly aspect of the classifier, application of KNN model suits a large spectrum of applications.

## Theoritical Background - Fundamentals and Design Considerations of K-Nearest Neighbors and its Parameters

KNN algorithm is a versatile and widely used machine learning algorithm that is primarily used for its simplicity and ease of implementation. It does not require any assumptions about the underlying data distribution. It can also handle both numerical and categorical data, making it a flexible choice for various types of datasets in classification and regression tasks. Underlying this effective and efficient algorithm are some significant parameters as mentioned below –

1. Methods of distance calculation:

There are a lot of different distance metrics available, however for the algorithm to work best on a particular dataset, it is important to choose the most appropriate distance metric. Some of the most widely used ones are as below –

Minkowski Distance – It is a metric intended for real-valued vector spaces. We can calculate Minkowski distance only in a space where distances can be represented as a vector that has a length and the lengths cannot be negative. There are a few conditions that the distance metric must satisfy:

Non-negativity: d(x, y) >= 0

Identity: d(x, y) = 0 if and only if x == y

Symmetry: d(x, y) = d(y, x)

Triangle Inequality: d(x, y) + d(y, z) >= d(x, z)

A mathematical equation with numbers and symbols

Description automatically generated

This above formula for Minkowski distance is in generalized form. The p value in the formula can be manipulated to give us different distances like:

p = 1, when p is set to 1, we get Manhattan distance

p = 2, when p is set to 2, we get Euclidean distance

Manhattan Distance – This distance is also known as taxicab distance or city block distance, because of the way this distance is calculated. The distance between two points is the sum of the absolute differences of their Cartesian coordinates. As mentioned earlier, the formula for Manhattan distance is achieved by substituting p=1 in the Minkowski distance formula –

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This distance is preferred over Euclidean distance when we have a case of high dimensionality.

Euclidean Distance – It is a measure of the true straight-line distance between two points in Euclidean space. It can be used by setting the value of p equal to 2 in Minkowski distance metric.

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Cosine Distance – This distance metric is used mainly to calculate similarity between two vectors. It is measured by the cosine of the angle between two vectors and determines whether two vectors are pointing in the same direction. Formula for the cosine distance is as follows –

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Using this formula, a value can be obtained conveying the similarity between the two vectors. Using this distance, we get values between 0 and 1, where 0 means the vectors are 100% similar to each other and 1 means they are not similar at all. In this project, cosine similarity distance metrics has been utilized for the classification using KNN.

Jaccard Distance – The Jaccard approach[5] looks at two data sets and finds the incident where both values are equal to 1. So, the resulting value reflects how many one-to-one matches occur in comparison to the total number of data points. It is extremely sensitive to small samples sizes and may give erroneous results, especially with very small data sets with missing observations. The formula[6] for Jaccard index is -

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Jaccard distance[7] is the complement of the Jaccard index and can be found by subtracting the Jaccard Index from 100%, thus the formula for Jaccard distance is - D(A,B) = 1 – J(A,B).

Hamming Distance - Hamming distance is a metric for comparing two binary data strings. While comparing two binary strings of equal length, hamming distance is the number of bit positions in which the two bits are different. The Hamming distance method looks at the whole data and finds when data points are similar or dissimilar one to one. It gives the result of how many attributes were different. This is used mostly when data is one-hot encoded, and it is required to find distances between the two binary vectors. For e.g., if two strings “ABCDE” and “AGDDF” of same length are present and it is required to find the hamming distance between these strings, then letter by letter in each string is checked and verified whether they are similar or not, like first letters of both strings are similar, then second is not similar and so on. At the end, it is seen that only two letters were similar and three were dissimilar in the given strings. Hence, the Hamming Distance here will be 3. It is to be noted that larger the Hamming Distance between two strings, more dissimilar will be those strings (and vice versa).

2. Selection of ‘K’ value:

The choice of the k value in the k-Nearest Neighbors (KNN) classifier is a crucial parameter that significantly influences the model's performance. The value of k represents the number of nearest neighbors considered during the classification process. A smaller k value, such as k=1, leads to a more flexible model that can be sensitive to noise in the data but may overfit. On the other hand, a larger k value, such as k=5 or k=10, provides a smoother decision boundary, offering more robustness to noise. The selection of an optimal k value often involves a trade-off between model sensitivity and generalization. Cross-validation techniques, such as k-fold cross-validation, can be employed to assess the model's performance across different k values and help determine the most suitable one for a given dataset. Experimentation and testing various k values are essential to strike the right balance between bias and variance, ensuring an effective and accurate KNN classification model.

3. Softmax algorithm:

The Softmax function is a function that turns a vector of K real values into a vector of K real values that sum to 1. The input values can be positive, negative, zero, or greater than one, but the Softmax transforms them into values between 0 and 1, so that they can be interpreted as probabilities. If one of the inputs is small or negative, the Softmax turns it into a small probability, and if an input is large, then it turns it into a large probability, but it will always remain between 0 and 1. Many multi-layer neural networks end in a penultimate layer which outputs real-valued scores that are not conveniently scaled and which may be difficult to work with. Here the Softmax is very useful because it converts the scores to a normalized probability distribution, which can be displayed to a user or used as input to other systems. For this reason, it is usual to append a Softmax function as the final layer of the neural network.

## Hierarchical Temporal Memory (HTM)

The HTM algorithm is based on the well understood principles and core building blocks of the Thousand Brains Theory. In particular, it focuses on three main properties: sequence learning, continual learning, and sparse distributed representations. Compared to Recurrent Neural Networks (RNNs), HTMs have a more complex neuron model. HTMs don’t employ back-propagation but a simple and local unsupervised Hebbian-learning rule. Moreover, they are based on very sparse activations and neuron connectivity[8].

# **IMPLEMENTATION**

The KNN classifier is used within the experiment to learn sequences and predict future elements based on the learned patterns. KNN is used alongside HTM to aid in predicting values based on the active cells and winners obtained from HTM components such as spatial pooler and temporal memory. The KNN classifier learns patterns derived from HTM activations and tries to predict the next elements in the sequences. This section of the paper describes in detail the important methods of the code and the logic with which they are implemented.

1. Learn

*public void Learn (TIN input, Cell[] cells)*

The Learn method is a crucial component of the K-nearest neighbors (KNN) classifier, serving to enhance the model's understanding of new input patterns. Initially, it extracts the classification label corresponding to the provided input, utilizing the ***GetClassificationFromDictionary*** method. Subsequently, the method transforms the array of Cell objects (cells) into an array of integer indices, capturing the specific indices associated with each cell. The final step involves updating the internal models of the KNN classifier through the ***UpdateModels*** function. This function, in turn, ensures that the model incorporates the latest information by associating the obtained classification label with the array of cell indices.

2. GetPredictedInputValues

*public List<ClassifierResult<TIN>> GetPredictedInputValues(Cell[] unclassifiedCells, short howMany = 1)*

The ***GetPredictedInputValues*** method in the KNN classifier is responsible for predicting input values based on the distances between unclassified cells and the stored sequences in the model. To begin with, it checks if there are any unclassified cells, and if not, it returns an empty list of ClassifierResult<TIN>

*if (unclassifiedCells.Length == 0)*

*return new List<ClassifierResult<TIN>>();*

The method then extracts the indices of the unclassified cells and initializes a DefaultDictionary named mappedElements to store distances and classifications.

*var unclassifiedSequences = unclassifiedCells.Select(cell => cell.Index).ToArray();*

*var mappedElements = new DefaultDictionary<int, List<ClassificationAndDistance>>();*

For each model in the internal dictionary of models, the method iterates through the stored sequences associated with that model. It calculates the distances between these sequences and the indices of the unclassified cells using the ***GetDistanceTableforCosine*** method. The resulting distances are then added to the mappedElements dictionary, where each key represents an index of an unclassified cell, and the value is a list of ClassificationAndDistance objects.

After populating mappedElements, the method sorts the values (distances) within each list according to their magnitude. Finally, the method calls the ***SelectBestClassification*** function to determine the best classifications based on similarity scores and weighted votes. The ***SelectBestClassification*** method combines normalized weighted votes and overlap scores, orders them by similarity scores, and returns a list of ClassifierResult<TIN> representing the predicted input values. The number of predictions returned is determined by the ‘howMany’ parameter, with the default set to 1.

*foreach (var mappings in mappedElements)*

*mappings.Value.Sort();*

*return SelectBestClassification(mappedElements, howMany, neighbors);*

3. GetDistanceTable

*private Dictionary<int, List<ClassificationAndDistance>> GetDistanceTable(int[] classifiedSequence, int[] unclassifiedSequence)*

The ***GetDistanceTable*** method calculates distances between a classified sequence and an unclassified sequence. For each index in the unclassified sequence, it computes the shortest distance using the ***LeastValue*** method.

*foreach (var unclassifiedIdx in unclassifiedSequence) {*

*var shortestDistance = LeastValue(classifiedSequence, unclassifiedIdx);*

The distances are stored in a dictionary where each key represents an index from the unclassified sequence, and the associated value is a list of ClassificationAndDistance objects containing the classification label ("Classification") and the respective shortest distance. The method then returns this distance table.

## 4. ComputeCosineSimilarity

*private double ComputeCosineSimilarity(HashSet<int> classifiedSet, HashSet<int> unclassifiedSet)*

The ***ComputeCosineSimilarity*** method calculates the cosine similarity between two sets represented by HashSet<int> instances (classifiedSet and unclassifiedSet). It starts by computing the dot product of the two sets, i.e., the count of common elements. Then, it determines the lengths of both sets. To avoid division by zero, it checks for edge cases where either set has zero length and returns 0.0 in such situations. Finally, it calculates the cosine similarity using the dot product and the lengths of the sets, providing a measure of similarity between the classified and unclassified sets. The result is a double value representing the cosine similarity, with 1.0 indicating perfect similarity and 0.0 indicating no similarity.

Similar to ***GetDistanceTable*** method discussed earlier, ***GetDistanceTableforCosine*** is also implemented to compute the cosine similarity between a classified sequence and an unclassified sequence and generates a distance table.

5. SelectBestClassification

*Public List<ClassifierResult<TIN>> SelectBestClassification(Dictionary<int, List<ClassificationAndDistance>> mapping, int howMany, int numberOfNeighbors)*

The ***SelectBestClassification*** method is one of the most significant components in the K-nearest neighbors (KNN) classifier for determining the most suitable classifications based on calculated similarity scores and weighted votes. The method initializes three dictionaries—weightedVotes, overlaps, and similarityScores—to store information regarding weighted votes, overlaps, and final similarity scores, respectively. Each classification key in the internal models is assigned initial values within the overlaps dictionary, and the weightedVotes dictionary is set to zero for each classification, initializing them for subsequent calculations.

The method then iterates through the provided mapping, which contains distance information between unclassified sequences and stored sequences from various models. For each set of coordinates in mapping, it selects the top 'numberOfNeighbors' neighbors and calculates votes based on distances. If the distance is zero, indicating an exact match, the corresponding overlap count is incremented, otherwise, weighted votes are computed inversely proportional to the distance.

*if (value.Distance == 0)*

*{*

*overlaps[value.Classification]++;*

*}*

*else*

*{*

*weightedVotes[value.Classification]+=1.0/value.Distance;*

*}*

Following the vote calculation, the method proceeds to normalize the weighted votes to ensure a balanced contribution from each classification. The normalization is performed by dividing each weighted vote by the maximum weighted vote. Additionally, similarity scores based on overlaps are computed, representing the proportion of instances where exact matches occurred.

Finally, the normalized weighted votes and overlap scores are combined to yield the overall similarity scores. The method orders these scores in descending order to facilitate the final decision-making process. The results are then transformed into a list of ClassifierResult<TIN> instances, each containing the predicted input, similarity score, and the count of overlapping bits. The final list is limited to the specified number (howMany) of best predictions, which is then returned by the method. ***SelectBestClassification*** is instrumental in consolidating and evaluating the various factors to arrive at the most suitable predictions in the KNN classification process.

6. PredictWithSoftmax

*Public List<ClassifierResult<TIN>> PredictWithSoftmax(Cell[] unclassifiedCells, short howMany = 1)*

The ***PredictWithSoftmax*** method represents an extension of the K-nearest neighbors (KNN) classifier by incorporating the Softmax algorithm to predict classifications for a given set of unclassified cells. It begins by checking if there are any unclassified cells; if not, it promptly returns an empty list. Subsequently, it extracts the indices of the unclassified cells and initializes a dictionary called mappedElements using the DefaultDictionary<int, List<ClassificationAndDistance>> structure, which will store distances and classifications.

The method iterates through each model in the internal models dictionary, which represents the pre-learned sequences and their corresponding classifications. For each sequence in a model, it calculates the distances between the stored sequence and the unclassified sequences using the GetDistanceTableforCosine method. The resulting distances and classifications are then added to the mappedElements dictionary.

*var distanceTable = GetDistanceTableforCosine(sequence, unclassifiedSequences);*

*foreach (var kvp in distanceTable)*

*{*

*if (!mappedElements.ContainsKey(kvp.Key))*

*{*

*mappedElements[kvp.Key] = new List<ClassificationAndDistance>();*

*}*

Following this, the distances in mappedElements are sorted to ensure a consistent ordering. Subsequently, Softmax weights are computed for each class based on the distances stored in mappedElements using the ***CalculateSoftmaxWeights*** method, introducing a softness parameter of 0.5. The Softmax function is then applied to these weights through the Softmax method, generating probabilities for each class.

*var softmaxWeights = CalculateSoftmaxWeights(mappedElements, 0.5);*

*var softmaxProbabilities = Softmax(softmaxWeights);*

The method creates a list of ClassifierResult<TIN> instances, where each instance contains the predicted input, calculated similarity (using Softmax probability as the similarity score), and any additional relevant information. Finally, the list is limited to the specified number (howMany) of best predictions, and the resulting predictions are returned by the method.

# **REFERENCES**

[1] Zhongheng Zhang, <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4916348/>, June, 2016

[2] Gongde Guo, Hui Wang, David A. Bell, Yaxin Bi, KNN Model-Based Approach in Classification, <https://www.researchgate.net/publication/2948052_KNN_Model-Based_Approach_in_Classification>, August 2004

[3] Manish Suyal, Piyush Goyal, A Review on Analysis of K-Nearest Neighbor Classification Machine Learning Algorithms based on Supervised learning, Department of CA & IT, SGRR University, Uttarakhand, India, 18 July 2022

[4] Kashvi Taunk; Sanjukta De; Srishti Verma; Aleena Swetapadma, A Brief Review of Nearest Neighbor Algorithm for Learning and Classification, IEEE publications, 16 April 2020

[5] Agresti A, Categorical Data Analysis. John Wiley and Sons, New York, 1990.

[6] Dodge Y, The Concise Encyclopedia of Statistics. Springer, 2008.

[7] Wheelan, C, Naked Statistics. W. W. Norton & Company, 2014

[8] Vincenzo Lomonaco, <https://www.numenta.com/blog/2019/10/24/machine-learning-guide-to-htm/>, Oct 24, 2019