Introduction to Machine Learning: Work 2
Classification with Lazy Learning and SVM

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Abstract

This is the abstract. Summarize the purpose, methods, and main findings of the study.

1 Introduction

Introduce the problem, background, and significance of the study.

2 Methodology

Describe the datasets and outline each method applied.

2.1 Datasets

Briefly describe Dataset 1 and Dataset 2.

2.2 K-Nearest Neighbors (KNN)

The implementation of the KNN algorithm is encapsulated in the `KNNAlgorithm` class. It allows the selection of different distance metrics, weighting methods, and voting policies to classify test instances using their nearest neighbors. The methodology follows these three main components.

2.2.1 Hyperparameters

1. **k:**
    - The number of Nearest Neighbors to be considered in the algorithm. This can take any integer value. In our study, we have employed values $1, 3, 5$ and 7.

2. **Distance Metrics:**

   - **Euclidean Distance**: Calculates the root of the sum of squared differences between feature values. It is commonly used for continuous data and defined as:

$$d(x, y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

   - **Manhattan Distance**: Computes the sum of absolute differences between feature values, suitable for both categorical and continuous data. It is defined as:

$$d(x, y) = \sum_{i=1}^{n} |x_i - y_i|$$

   - **Clark Distance**: Accounts for proportional differences between feature values, enhancing interpretability for attributes with varying scales. It is computed as:

$$d(x, y) = \sqrt{\sum_{i=1}^{n} \left(\frac{|x_i - y_i|}{x_i + y_i + \epsilon} \right)^2}$$

     where ϵ is a small constant to avoid division by zero.

3. **Weighting Methods:**

   - **Equal Weight**: Assigns equal importance to all features by setting each feature's weight to 1.
   - **Information Gain Weight**: Uses mutual information to assign weights based on each feature's information gain with respect to the class label.
   - **ReliefF Weight**: Computes feature relevance by evaluating differences between feature values of similar and dissimilar instances, adjusted by the specified number of neighbors.

4. **Voting Policies:**

   - **Majority Class**: Assigns the class based on the most common class label among the nearest neighbors.
   - **Inverse Distance Weighted**: Weights each neighbor's vote by the inverse of its distance, giving more influence to closer neighbors. The vote for class y is calculated as:

$$\text{Vote}_y = \sum_{i \in \mathcal{N}_y} \frac{1}{d(q, x_i)}$$

     where $\mathcal{N}_y$ represents neighbors with class y.

- **Shepard's Work**: Similar to the Inverse Distance Weighted policy, except that it applies exponential decay to the distance (instead of the inverse), allowing stronger influence from closer neighbors. The vote for class y is:

$$\text{Vote}_y = \sum_{i \in \mathcal{N}_y} e^{-d(q,x_i)}$$

This structure enables flexible configurations for analyzing the performance of the KNN algorithm across different datasets and hyperparameter values.

2.2.2 Results extraction

To systematically evaluate the KNN model configurations, the following procedure is followed to extract results for each of the 2 data sets, in order to later perform an statistical analysis:

1. **Data Preparation**: Each fold of the dataset is loaded, split into training and testing sets. Features may also be weighted using different weighting methods to analyze their impact on model performance. This is applied as a pre-processing step in order to optimize execution times.

2. **Parameter Configuration**: A comprehensive set of values for the KNN hyperparameters is defined. These combinations reflect various ways to tune the KNN model.

3. **Model Evaluation**: For each fold and parameter combination, the KNN model is trained on the training data and evaluated on the test data. This step yields the following metrics: accuracy, execution time, and F1-score. Together, these measure the model's effectiveness and efficiency.

4. **Results Compilation**: The performance metrics for each parameter combination and fold are recorded in a structured format. These results are saved as a dataset that summarizes the outcomes of all evaluations, forming a basis for analysis.

5. **Statistical Analysis**: After results are compiled across all configurations and folds, statistical analysis is performed to identify the best-performing configurations. This analysis helps determine the most reliable and effective parameter settings for accurate and efficient KNN classification. We will discuss our results in Section 3.

2.3 Support Vector Machine (SVM)

Describe the SVM approach.

2.4 Reduction Methods

In this section, we briefly describe reduction techniques employed for instance-based learning. We use a simple 2D dataset for illustrative purposes.

2.4.1 GCNN

The Generalized Condensed Nearest Neighbor (GCNN) algorithm is an extension of the traditional Condensed Nearest Neighbor (CNN) method, which incorporates adaptive prototype learning approach. This is an **undersampling** technique which try to find a subset of prototypes $U \subseteq X$, where $X = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ is our dataset, that correctly represents our data. This is specially beneficial for unbalanced datasets. The main idea behing CNN is to select prototypes that *absorbe* points that can be represented using that protype. Let's break down the steps for this method:

1. **Prototype selection:** In this step we need to select a prototype for each class. So for each class c_j, let $X_j = \{(x, y) : y = c_j\}$ be all the elements of this class. We will select as a prototype x_j^* that is the nearest neighbor of most points of its class, thus it will influence the most points in any KNN. i.e. :

$$x_j^* = \arg\max_{x \in X_j} \left(\sum_{x' \in X_j \setminus \{x\}} \left(x = \mathrm{NN}_{X_j \setminus \{x'\}}(x')\right) \right)$$

   So we will have $U = \{x_j^* : j = 1, \ldots, m\}$ and we will denote as U_j all the prototypes of class c_j.

2. **Absorbtion:** This is one of the key differences with CNN, first let define $\delta_n = \min_{\{(x_i,y_i),(x_j,y_j) \in X : y_i \neq y_j\}} \left(\|x_i - x_j\|\right)$, for every point x_i let $p = \arg\min_{x \in U_j} \left(||x - x_i||\right)$ and $q = \arg\min_{x \in (U \setminus U_j)} \left(||x - x_i||\right)$ be the nearest protoypes of the same class and other class respectively. We will absorb x_i if it satisfy the following condition:

$$\|\mathbf{x} - \mathbf{q}\| - \|\mathbf{x} - \mathbf{p}\| > \rho\delta_n, \quad \rho \in [0, 1).$$

   With CNN being $\rho = 0$, this means that if the x_i's closest prototype is of its class, it will be absorbed. ρ variables just introduces a slack for this decission illustrated in **Figure** 1

3. **Prototype Augmentation:** If there are still points that haven't been absorbed for class c_j, we will repeat the prototype selection but only taking into account unabsorbed points and then go to step 2 again. If all points have been absorved we finish the process.

In **Figures** 2 and 3 we illustrate the effect of this method in a specially constructed dataset where we can clearly see it with ρ varying froom 0 to 1.

2.4.2 EENTH

This subsection outlines the Elimination Editing with Nearest-neighbor Threshold (EENTH) method [1]. This approach uses a modified k-NN rule, integrating probability-based decisions for instance elimination. The main steps are outlined below.

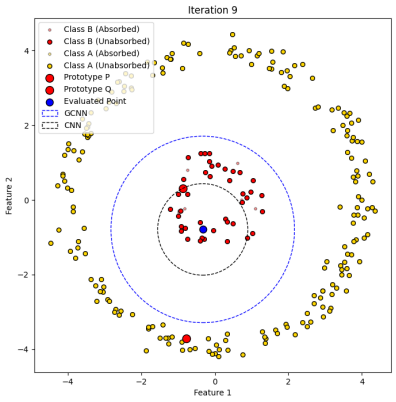
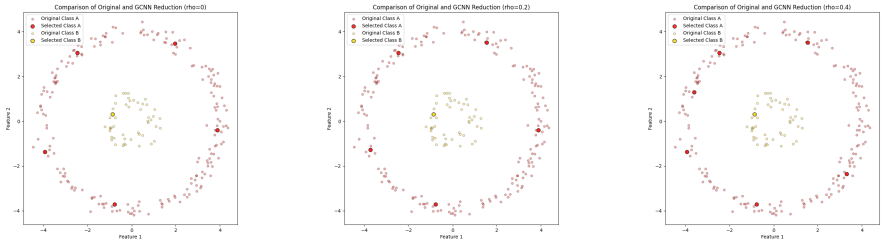


Figure 1: Effect of Rho in GCNN Illustrated



(a) $\rho = 0$ (b) $\rho = 0.2$ (c) $\rho = 0.4$

Figure 2: GCNN illustration $\rho = 0.6, 0.8, 1$

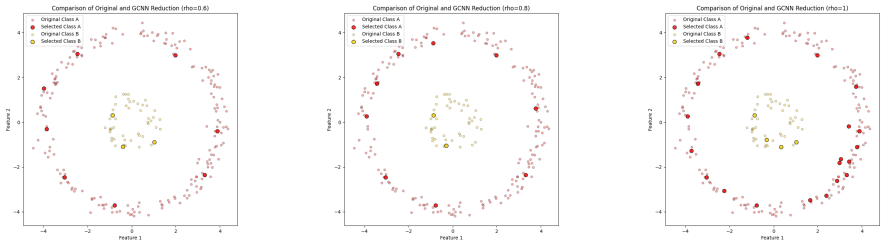
1. **Probability-based Classification**: For each instance x, calculate the probability $p_i(x)$ of x belonging to each class i based on its k-nearest neighbors. Probabilities are weighted inversely by the distance to each neighbor and normalized:

$$p_i^j = \frac{|\{x_k \in NN_k(x) : y_k = j\}|}{k} \tag{1}$$

$$P_i(x) = \sum_{j=1}^{k} p_i^j \frac{1}{1 + d(x, x^j)} \tag{2}$$

$$p_i(x) = \frac{P_i(x)}{\sum_{j=1}^{M} P_j(x)} \tag{3}$$

2. **Thresholding**: Define a threshold μ to refine classification, we will denote



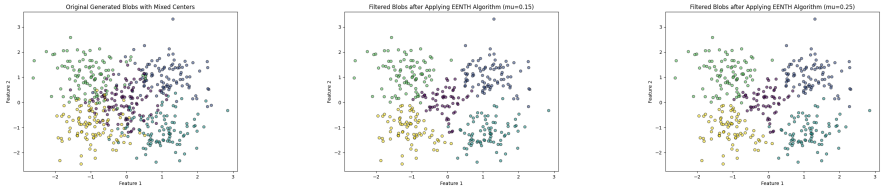
(a) $\rho = 0.6$ (b) $\rho = 0.8$ (c) $\rho = 1$

Figure 3: GCNN illustration $\rho = 0.6, 0.8, 1$

as $p(x)$ the highest probability. Instances near decision boundaries, where $p(x) < \mu$, are identified as candidates for removal.

3. **Elimination**: If an instance x does not match the class with the highest probability, or if its highest class probability falls below μ, it is removed from the dataset, resulting in an edited set $S \subseteq X$.

The EENTH method thus provides a balance between retaining instances with high classification confidence and discarding uncertain instances near decision boundaries. Best values for μ are dependent on the dataset, In **Figures ??** we illustrate the results for μ varying from 0.15 to 0.85 taking 5 neighbors into account.

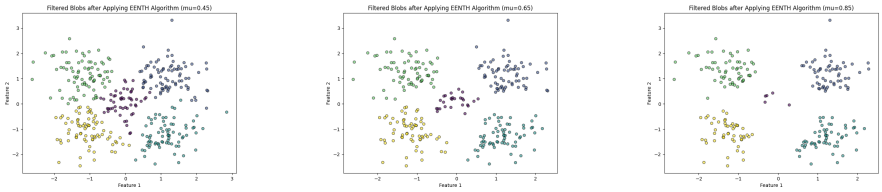


(a) Original (b) $\mu = 0.2$ (c) $\mu = 0.4$

Figure 4: Illustration of dataset after applying EENTH method with μ values 0.15 and 0.25.

2.4.3 DROP3

In this subsection, we describe the basic concepts of the third method in the Decremental Reduction Optimization Procedure (DROP) family, as presented in Section 3 of Wilson et al. [3]. Although we will not delve into every detail, we describe the main ideas of the algorithm and illustrate them on D_1. See **Figure** 6.



(a) $\mu = 0.45$ (b) $\mu = 0.65$ (c) $\mu = 0.85$

Figure 5: EENTH illustration $\mu = 0.45, 0.65, 0.85$

1. **Remove noise**: The first step is to remove noisy instances using Edited Nearest Neighbor (EEN) [2], where any instance misclassified by its k-nearest neighbors is removed. The outcome of applying this technique is shown in **Figure** 7, where noise has been removed. We denote the reduced dataset as $T \subseteq D_1$.

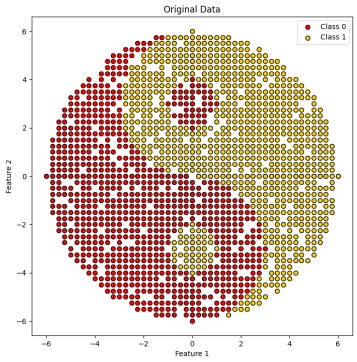


Figure 6: Original Dataset

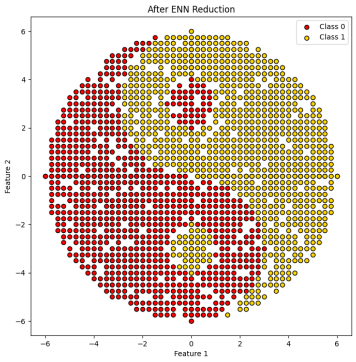


Figure 7: Effect of EEN

2. **Sort points**: The next step is to prioritize removing points that are farthest from the decision boundary. For each point $x_i \in S$ with class y_i, we compute the distance to the nearest point with a different class, denoted as $x_j \in D$ such that $y_j \neq y_i$ and $\nexists x_k : |x_k - x_i| < |x_j - x_i| \wedge y_i \neq y_k$.

3. **Delete points**: Let $S = T$. Starting with the points farthest from the boundary, we check if any associated points (points that have x_i as a neighbor) a_j receive more votes for their correct class with x_i as a neighbor (denoted as with) or if they would be classified correctly if x_i were removed (denoted as without). If without $>$ with, we remove x_j from S, resulting in $S' = S \setminus \{x_j\}$.

4. **Selecting neighbors**: A key distinction between DROP1 and DROP2 is

that DROP1 removes points that are removed from the dataset from the list of associates while DROP2 doesn't.

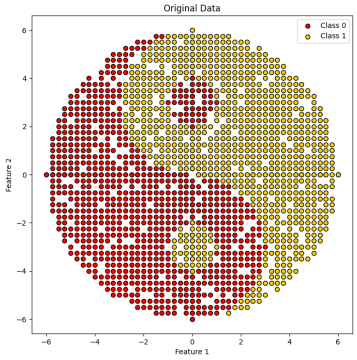


Figure 8: Original Dataset

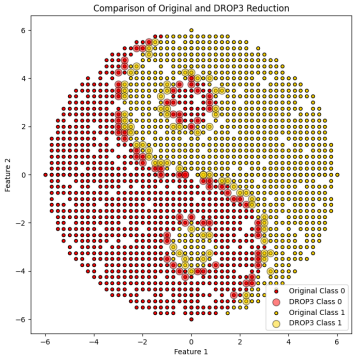


Figure 9: Effect of DROP3

3 Results

Present the findings and the conclusions of the statistical analysis. For each technique, we will separately discuss the results obtained with each of the 2 datasets. It is important to note that in the study of each dataset we have considered each of the 10 folds as separate datasets in order to perform the statistical analysis. This consideration is sub-optimal, but necessary due to the time and hardware constraints.

3.1 KNN Results

We have evaluated the total 108 different KNN model configurations that can be achieved by assigning the different values available to each of the hyper-parameters of the algorithm (k, distance metric, weighting method and voting policy).

We have trained and tested each of the KNN configurations on the 10 folds of each of the 2 datasets, and stored their achieved accuracy, time and F1 scores in 2 separate CSV files (one per dataset). In the following Subsections, we will discuss some metrics extracted from these results, and we will perform multiple statistical analyses in order to determine whether there are significant differences between the models or not.

3.1.1 Hepatitis

First of all, we summarize the obtained results in a pairplot matrix (Figure 10). Each row and column of the matrix represents a hyperparameter, and

the diagonal displays the accuracy histograms for each of the values of the corresponding hyperparameter. Meanwhile, the lower and upper triangles of the matrix display, respectively, the average accuracy and time heatmaps over the folds for each pairwise configurations of the 2 corresponding hyperparameters. With this kind of pairplot we get useful insight into the relationships betweem hyperparameters. We can see a clear trend towards better performance as the value of k goes up; however, this is a preliminary visualization and we cannot extract any real definitive conclusions.

Next, we filter out the top 10 performing models (based on average accuracy over the folds) and we perform a statistical analysis on them to try to find significant differences. After filtering the top 10 models, we apply a Friedman test on their accuracies over the 10 folds, with the null-hypothesis being that there is no significant difference between the models. From the Friedman test we obtain a p-value of **0.9997**, which overwhelmingly supports the null-hypothesis and indicates that there are not any statistically significant differences between the top 10 models.

Since we could not find a model that stands out over the rest with the standard statistical analysis over individual models, we now aim to at least find some indication as to which hyperparameter values are more prominent in succesful models. In order to do this, we performed 4 separate statistical tests by grouping the models according to their configuration of each of the hyperparameters. In other words, we applied a Friedman test to each of the hyperparameters to try to find significant differences between each of their possible values. The obtained p-values for each of the 4 Friedman tests can be seen in Table 1.

k	**Distance metric**	**Weighting Method**	**Voting Policy**
0.2071	0.2765	0.1211	nan

Table 1: Friedman test p-values per hyperparameter.

If we set a level of significance of $\alpha = 0.15$ (which is already a relatively high value), we can only find significant differences between the different weighting methods. Note that the "nan" value in the test over the voting policy means that the ranks across the 4 different voting policies are identical, and therefore the Friedman test cannot be applied. This supports the null-hypothesis of not finding significant differences between the voting policies. We can see the results in Table 2.

Finally, we perform a post-hoc test on the weighting methods in order to further study the significant differences that we have found. In this case, the most appropriate post-hoc test to perform is the Bonferroni test with a control, since there is a clear "standard" choice of weighting method, which is Equal Weights, and we want to find if the other 2 weighting methods have any advantage over it.

Considering the calculated p-values, we can conclude that, with a significance level of $\alpha = 0.15$, we find statistically significant differences between the ReliefF weighting method and the control (Equal Weights), and we do not have strong

	p-value	Difference in accuracy (%)
Information Gain	0.2138	-7.7961%
ReliefF	0.1358	-3.3461%

Table 2: Results of the Bonferroni post-hoc test

enough evidence to support the same claim for the Information Gain method. Looking at the average difference in accuracy percentage, we see that the ReliefF weighting method usually performs worse than Equal Weights on the Hepatitis dataset, and therefore we can conclude that it is siginificantly worse to utilize it instead of the standard Equal Weights when classifying samples of this dataset.

Before going to the next section, it is important to note that, since we did not find significant differences between the top performing KNN models, we can assume that all of the top models have statistically the same performance on the Hepatitis dataset. Hence, for simplicity's sake, we will take the one with the highest average accuracy rate (0.8519) in order to perform later tests of comparison between models, and between reduction methods. This model has a k value of 7, the Manhattan Distance, the Equal Weight method, and the Majority Class voting.

3.1.2 Mushroom

For the Mushroom dataset we will follow essentially the same steps as we did for the Hepatitis dataset, starting with visualizing the results in a pairplot matrix (Figure 11). Interestingly, in this case we observe the opposite trend on the values of k as we did for the Hepatitis dataset, which indicates better perfomance of lower values of k this time. We can also see a tendency towards slightly better accuracy when using the Clark distance; however, we also observe extreme values of the computation time for said distance metric.

As we did before, we proceed with a Friedman test to try to find significant differences among the top performing models. This time we get a p-value of **nan**, which indicates that there is absolutely no difference in the ranks between the top 10 models. When observing the results, we find that all of the 10 models have an average accuracy of 1.0, which means that they all perfectly classify all of the test samples across the 10 folds of the Mushroom dataset. The only conclusion that we can take from this result is that the Mushroom dataset is not complex enough to show any difference in performance between these model configurations.

Next, we perform a statistical test on the hyperparameters in order to find significant differences between their possible values. The results can be found in Table 3.

k	Distance metric	Weighting Method	Voting Policy
nan	nan	0.0000	nan

Table 3: Friedman test p-values per hyperparameter.

We see that the Friedman test cannot find any performance differences whatsoever between the different values of k, distance metric and voting policy. On the other hand, it is interesting to find that the p-value is **0.0000** for the weighting method, which essentially *guarantees* (due to numerical approximation of the p-value) significant differences between the various weighting methods.

After applying the Bonferroni post-hoc test on the weighting methods, we get the results displayed on Table 4.

	p-value	**Difference in accuracy (%)**
Information Gain	0.0039	-8.0502%
ReliefF	0.0039	-48.2029%

Table 4: Results of the Bonferroni post-hoc test

With these results, we can state that there is very strong evidence supporting that there is indeed significant differences between the Equal Weights method and the other 2; since even with a significance level of $\alpha = 0.01$ we would reject the null-hypothesis. Looking at the average difference in accuracy percentage, we can see that both weighting methods show poorer average performance than the Equal Weights, and therefore it is detrimental to use them over the "standard" weighting method.

Similarly as with Hepatitis dataset, we could not find significant differences between the top performing models upon the Mushroom dataset. Therfore, for future comparisons we could utilize any of the top 10 models (all of them have accuracy rate of 1), so we choose one that seems to have the simplest configuration of hyperparameters: a k value of 1, the Euclidean Distance, the Equal Weight method, and Majority Class voting.

3.2 SVM Results

Describe the SVM results.

3.3 KNN Reduction Results

Discuss the outcomes for KNN with reduction methods.

3.3.1 Hepatitis

Hepatitis results.

3.3.2 Mushroom

Mushroom results

3.4 SVM Reduction Results

Describe the SVM results with reduction methods.

4 Discussion

Interpret the results, relate to previous work, and discuss implications.

5 Conclusion

Conclude the report.

References

[1] Fernando Vázquez, Josep Sánchez, and Filiberto Pla. A stochastic approach to wilson's editing algorithm. pages 35–42, 01 2005.

[2] D. L. Wilson. Asymptotic properties of nearest neighbor rules using edited data. IEEE Transactions on Systems, Man, and Cybernetics, 2(3):408–421, 1972.

[3] Dennis R. Wilson and Tony R. Martinez. Reduction techniques for instance-based learning algorithms. Machine Learning, 38(3):257–286, 2000.

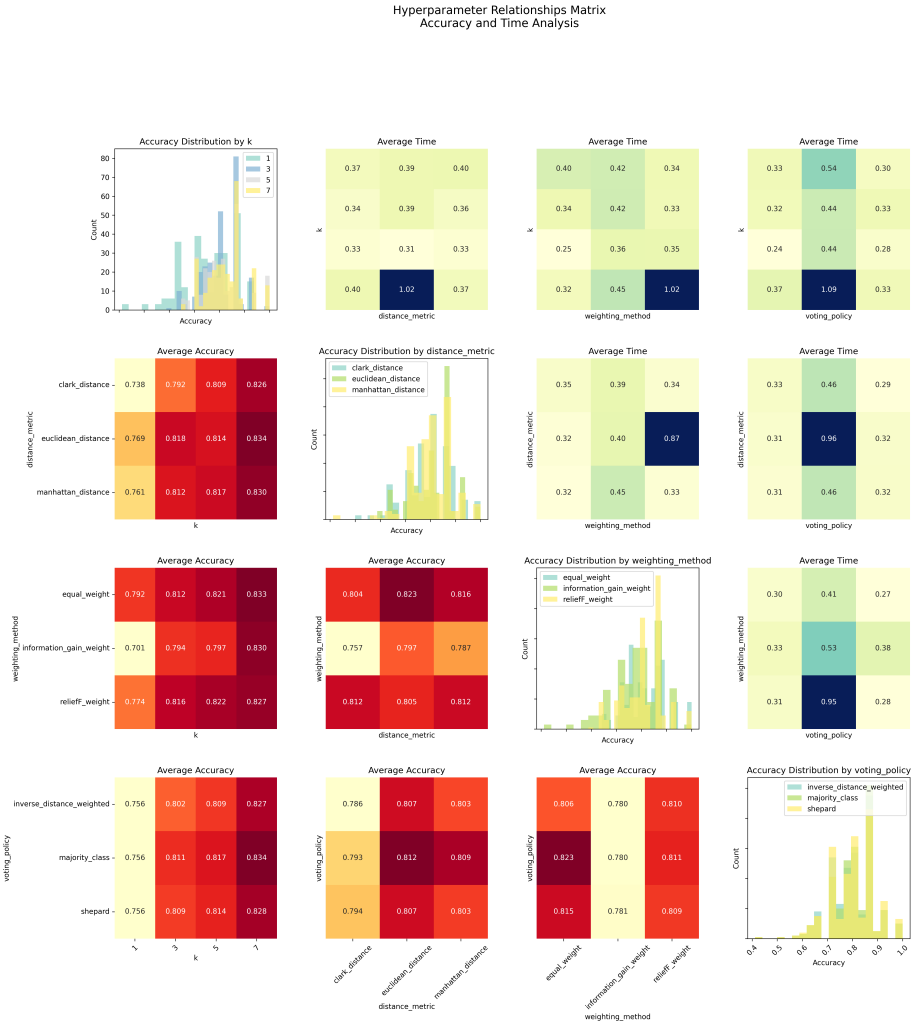


Figure 10: Hepatitis pairplot matrix summary

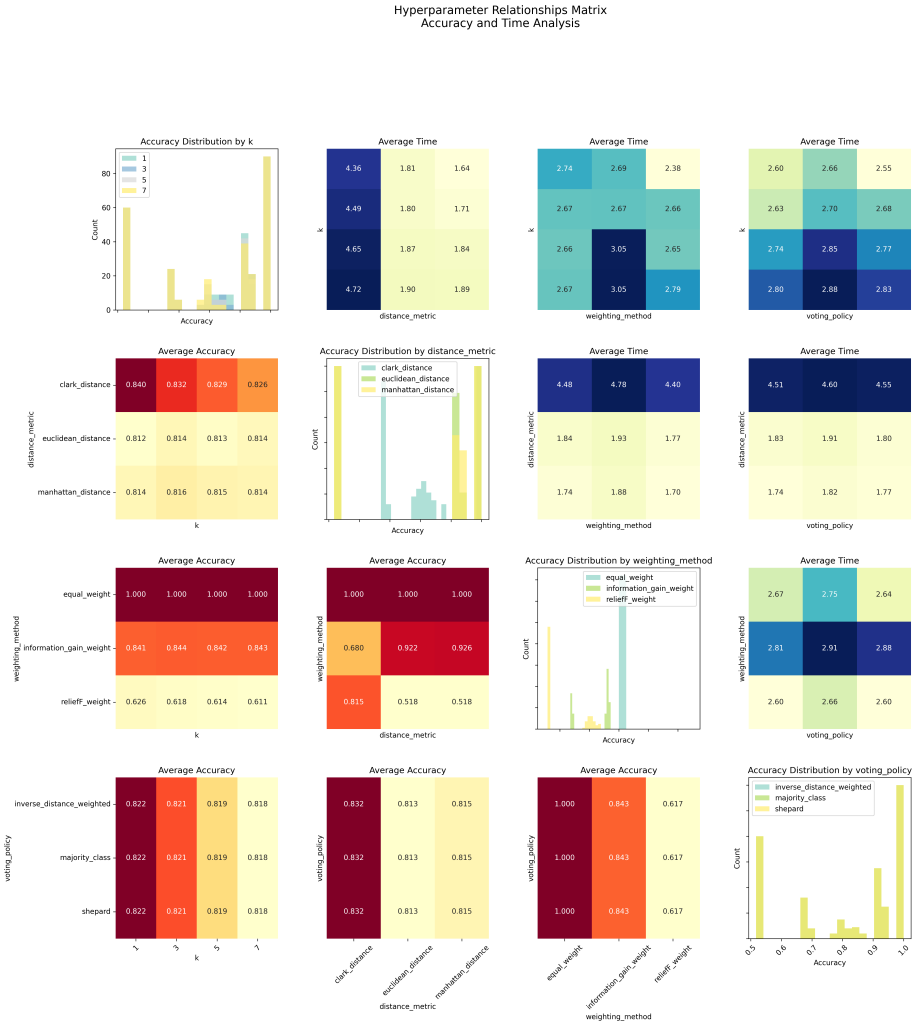


Figure 11: Mushroom pairplot matrix summary