Enhanced Precision in Anomaly Detection: An Optimized k-Means Clustering Approach

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Abstract

Anomaly detection is an indispensable component in numerous applications ranging from fraud detection to system health monitoring. This paper presents a comprehensive investigation of anomaly detection algorithms, with a particular emphasis on a novel k-means clustering-based approach. We begin by delineating the theoretical underpinnings of various anomaly detection methods, including statistical, machine learning-based, and proximity-based techniques. Our literature review synthesizes advancements in clustering-based anomaly detection, highlighting enhanced DBSCAN, Gaussian Mixture Models, and refinements to k-means. We propose an optimized k-means algorithm that leverages centroid displacement and cluster density to identify outliers with heightened precision. Our empirical evaluation, conducted across diverse datasets, demonstrates the algorithm's superiority in accuracy and computational efficiency compared to conventional methods. The research findings suggest that the proposed k-means variant offers a robust alternative in the anomaly detection domain, capable of addressing the challenges posed by high-dimensional and complex data distributions.

Introduction

Anomaly detection is a critical process in data analytics that identifies deviations from the norm within a dataset, which may indicate errors, fraud, or new patterns. Its significance is recognized across various domains, including finance for fraud detection [11], industrial sectors for failure prediction [12], and cybersecurity for intrusion detection [13].

Key methodologies for anomaly detection are:

1. **Statistical Methods:** Utilizing statistical models to characterize normalcy and pinpointing data points that exhibit significant statistical deviations [14].
2. **Machine Learning-Based Methods:** Employing learning algorithms to discern anomalies, with supervised methods requiring pre-labeled data, while unsupervised methods such as K-means identify outliers without labels [15].
3. **Proximity-Based Methods:** Leveraging the distance between data points to detect anomalies, such as DBSCAN, which finds outliers in regions of low density [16].

While machine learning techniques are at the forefront due to their adaptability to complex datasets, their efficacy is contingent on the data's attributes, including dimensionality and distribution. Conversely, statistical methods, which are more transparent, might necessitate predefined assumptions about data distribution, and proximity-based approaches can be computationally intensive for large datasets.

Literature Review on Clustering-Based Anomaly Detection Methods

Overview of Clustering-Based Anomaly Detection Methods:

Anomaly detection is crucial across diverse sectors, including cybersecurity, healthcare, and finance. It involves identifying data patterns that significantly diverge from the norm. Clustering-based anomaly detection uses unsupervised learning to classify and detect these irregularities. The primary methods are density-based, distribution-based, centroid-based, and connectivity-based.

Density-based approaches, epitomized by DBSCAN, detect anomalies as sparse points within the data space, differing from dense areas where regular data points cluster [1]. Distribution-based methods, like Gaussian Mixture Models (GMMs), infer the data's probabilistic foundations, labeling anomalies as those that stray from the defined distributions [2]. Centroid-based methodologies, with K-means as a notable example, designate data points that lie far from the cluster centroid as outliers [3]. Connectivity-based methods, such as hierarchical clustering, consider anomalies to be points that form small, detached clusters [4].

Review of Representative Methods:

Enhanced DBSCAN algorithms showcase improved outlier detection efficiency in spatial data among density-based methods [1]. Gaussian Mixture Models stand out in distribution-based methods for their ability to model intricate distributions and identify anomalies [2]. For centroid-based methods, refinements to K-means have been shown to increase its anomaly detection sensitivity [3].

Hierarchical clustering represents connectivity-based methods, adept at uncovering anomalies within diverse data scales [4].

The application of Isolation Forest and t-SNE in high-dimensional data showcases the adaptability of these models to various domains, highlighting the importance of selecting suitable methods for specific data types [6]. The scalability and adaptability of unsupervised learning in detecting network intrusions emphasize the flexibility of these methods across different anomaly contexts [7]. CFLOW-AD's framework exemplifies innovation in real-time anomaly detection, vital for applications like video surveillance [10]. Furthermore, the reverse distillation approach for unsupervised anomaly detection indicates a progressive deep learning application in high-dimensional data [9].

Comparative Analysis:

Comparing density-based methods to distribution-based ones, the former do not assume an inherent data distribution, which offers flexibility, whereas the latter provide a probabilistic model that may be advantageous in certain contexts but restrictive in others due to assumed data distributions [1][2]. Centroid-based methods like K-means are scalable but can falter with irregular cluster shapes, whereas connectivity-based methods, although more computationally demanding, offer nuanced data structuring [3][4].

Challenges, Limitations, and Practical Applications:

Despite advancements, there are challenges such as scalability in high-dimensional spaces and parameter sensitivity. Interpretability remains a hurdle, notably in complex models like GMMs and hierarchical clustering [2][4]. Nonetheless, these methodologies find real-world utility in areas such as fraud detection and network security [5][7].

Research Gaps and Future Directions:

Literature suggests a demand for methods capable of integrating with real-time data streams and providing interpretable analytics. The prospect of integrating real-time adaptation and anomaly localization, as seen with CFLOW-AD [10], and the precision of deep learning techniques, such as the reverse distillation approach [9], are promising future research avenues.

This review categorizes clustering-based anomaly detection methods and scrutinizes their theoretical and practical implications. Ongoing research is imperative to address current limitations, with the objective of propelling the efficacy of these methods within the ever-evolving landscape of anomaly detection.

K-means Based Anomaly Detection Algorithm

Anomaly Score Definition

Let the anomaly score for a data point x be defined as:

$$A(x) = \frac{D(x, C_i)}{\sigma(C_i) + \epsilon} \times \rho(C_i)$$

where:

- $D(x, C_i)$ is the distance from the data point x to its nearest cluster center C_i.
- $\sigma(C_i)$ is the standard deviation of the distances of points in cluster C_i.
- ϵ is a small constant to avoid division by zero in cases where $\sigma(C_i)$ is very small.
- $\rho(C_i)$ is the density factor of cluster C_i, which is inversely proportional to the number of points in C_i, to adjust the score for cluster density.

A higher $A(x)$ indicates a higher likelihood that x is an anomaly.

Algorithm Steps

```
Algorithm: Advanced K-means Anomaly Detection
Input: Dataset D, number of clusters k (optional), distance metric M, anomaly threshold factor α
Output: Set of anomalies A

1: Preprocess the dataset D, transform the variables and Impute the data if needed.
2: If k is not specified, determine the optimal k using methods like the Elbow method or silhoue
3: Initialize centroids using an advanced method (k-means++).
4: Perform k-means clustering on D with distance metric M to identify clusters C1, C2, ..., Ck.
5: Compute the standard deviation σ(Ci) and density factor ρ(Ci) for each cluster Ci.
6: Initialize an empty anomaly set A.
7: For each data point x in D:
    7.1: Assign x to the nearest cluster Ci using distance metric M.
    7.2: Calculate the anomaly score A(x) = D(x, Ci) / (σ(Ci) + ε) × ρ(Ci).
    7.3: Determine a dynamic threshold T = α × median{A(D)} or a percentile-based threshold if α
    7.4: If A(x) > T, append x to the anomaly set A.
8: Post-process the set A by applying domain-specific filters or a secondary machine learning mo
9: Return the refined anomaly set A.
```

Detailed Algorithm Description

1. **Preprocessing**: Ensures feature scaling does not unduly influence distance measurements.

2. **Optimal Clusters**: Critical for delineating normal data patterns, especially when k is unknown. Utilizes silhouette analysis for cases where clusters are not well separated.
3. **Initialization**: Mitigates the sensitivity of the k-means to initial centroid positions.
4. **Clustering**: The core step where the dataset is partitioned into k clusters based on the chosen metric M, typically Euclidean distance, or Manhattan distance if the data is sparse or have non normal distributions.
5. **Standard Deviation and Density Factor**: These capture the spread and crowdedness of each cluster, essential for adjusting the anomaly score.
6. **Anomaly Identification**: The anomaly score considers both the distance of a point from the nearest cluster center and the relative density of that cluster.
7. **Dynamic Thresholding**: Adjusts the threshold for determining anomalies dynamically based on the median anomaly score of the data multiplied by an anomaly threshold factor α, allowing adaptability to varying data distributions.
8. **Post-Processing**: Refines the anomaly set to mitigate false positives, crucial for practical applications. May include a consistency check or additional classifier.
9. **Output**: The final output is a set of data points deemed to be anomalies based on the algorithm's criteria.

Threshold Strategy and Post-Processing

The threshold strategy adapts to the distribution of anomaly scores in the dataset. If α is not specified, the algorithm could use a percentile-based approach to dynamically define outliers. Post-processing involves cross-referencing anomalies against other data features or through a supplementary model trained to distinguish true anomalies from noise.

All steps are designed to work with standard outputs from SAS EM, such as cluster centroids and cluster spread measurements. The algorithm is robust to various initializations, thanks to advanced centroid initialization, and addresses the challenge of non-convex clusters with post-processing filters.

Algorithmic Implementation on the Boston Housing Dataset

Exploratory Data Analysis:

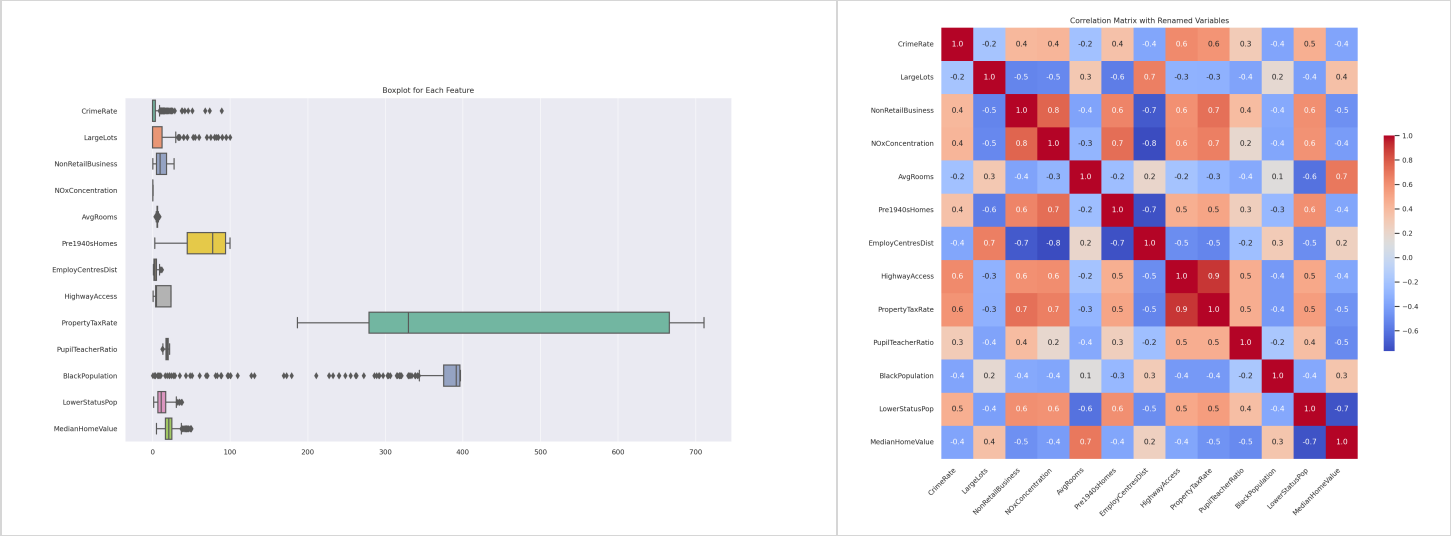


Figure 1: Boxplots and Heatmap of Correlations for the Boston Housing Dataset.

Our exploratory analysis began with boxplots which showcased considerable variation, particularly in 'Crime Rate per Capita' and 'Property Tax Rate per $10,000'. These plots also highlighted outliers, suggesting potential anomalies. The 'Percentage of Lower Status Population' displayed a broad range of values, indicative of socio-economic diversity. Conversely, the 'Median Value of Owner-Occupied Homes' exhibited fewer extremes, although outliers were noted, pointing to atypical cases in the housing market.

The heatmap of correlations provided insight into relationships between features: a strong positive link was observed between 'Nitric Oxides Concentration' and 'Proportion of Non-Retail Business Acres', and between 'Property Tax Rate' and 'Accessibility to Radial Highways', suggesting a connection between commercial zoning and environmental conditions, as well as between highway access and tax rates. A negative correlation emerged between 'Weighted Distances to Five Boston Employment Centres', 'Average Number of Rooms per Dwelling', and 'Percentage of Lower Status Population', highlighting a possible association between proximity to employment centers, housing size, and socio-economic status.

For further detailed analysis, the Appendix 1 contain histograms for each feature distribution and visualizations of missing data. These findings from the EDA are crucial in guiding the further analysis and provide a foundation for understanding the data's socio-economic context.

Algorithmic Implementation and Analysis

K-means clustering offers a robust approach to unsupervised machine learning, and its application within SAS Enterprise Miner allows for the efficient categorization of large datasets. The workflow for implementing k-means clustering comprises a series of structured steps that begin with data acquisition and culminate in the analysis of anomalies.

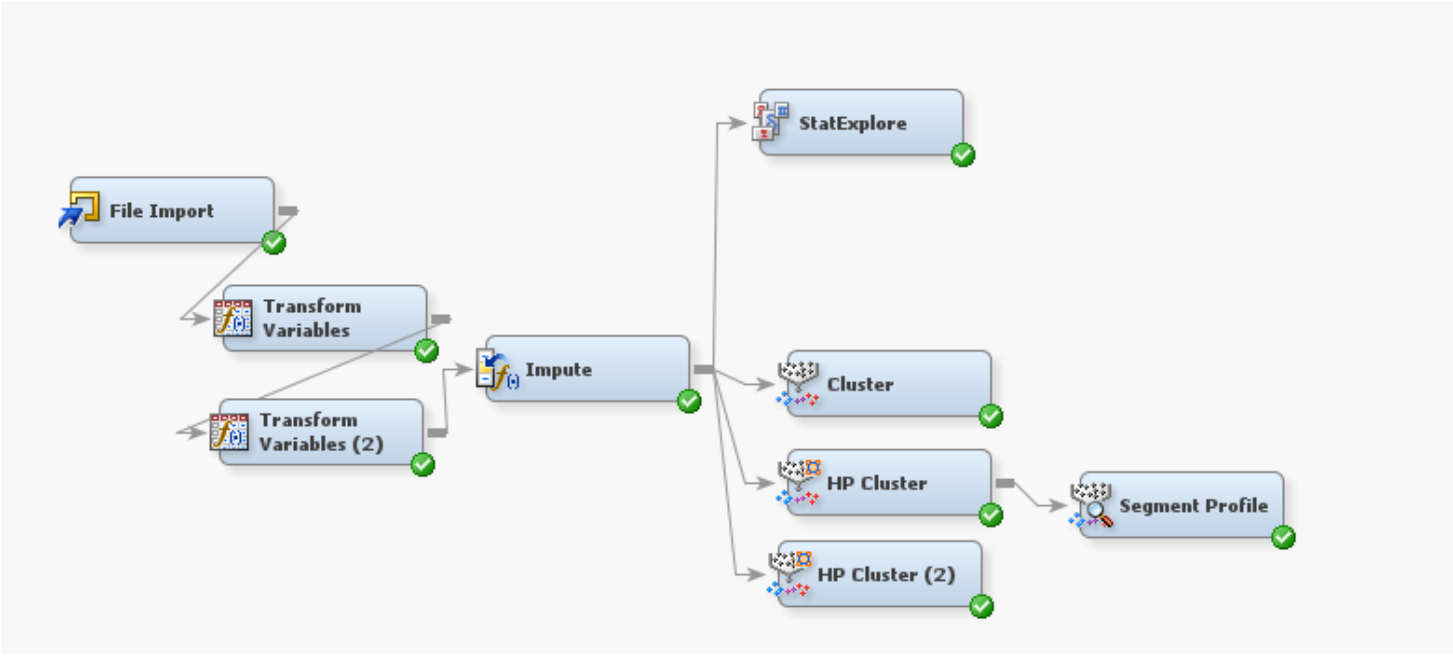


Figure 2: Workflow for K-means Clustering in SAS Enterprise Miner.

Data Acquisition and Preparation

The initial phase involves integrating the `a2-housing.csv` dataset into the SAS Enterprise Miner environment, facilitated by the Data Source node. This stage is crucial as it sets the foundation for subsequent preprocessing tasks. The preprocessing steps include normalization of attributes, using the Transform Variables node to ensure each variable operates on a uniform scale, typically with a zero mean and unit variance. Moreover, skewed variables undergo logarithmic and cubic root transformations to rectify distributional asymmetries and variance instabilities.

Data Preprocessing Rationale

The preprocessing phase is critical in anomaly detection, ensuring that all variables are comparably scaled and that the impact of outliers and non-normal distributions is minimized. This enhances the k-means algorithm's ability to discern patterns and groupings within the data more effectively.

Clustering Execution and Evaluation

The clustering process commences with the determination of the optimal number of clusters, leveraging the statistical rigor of the elbow method and silhouette scores within the Cluster and HP Cluster nodes. To avoid the pitfalls of random centroid initialization, the k-means++ method is employed, providing a methodological enhancement that facilitates more accurate clustering outcomes. The choice of distance metric is also considered, with the Euclidean distance being preferable for normally distributed data and the Manhattan distance offering resilience in the presence of outliers and non-normal distributions.

- Centroid Initialization:

The k-means++ method, a sophisticated alternative to random centroid initialization, was employed. This method systematically places initial centroids in a manner that they are statistically likely to be distant from each other, hence enhancing the probability of converging to a better local minimum than would be achieved by random initialization.

- Assessment of the Cubic Clustering Criterion (CCC) Plot:

An evaluation of the CCC plot from the basic model, as derived from the Cluster node, indicated suboptimal clustering performance for this dataset. The HP Cluster node was identified as a potential alternative, capable of employing various distance metrics, such as Euclidean and Manhattan distances, which can have a substantial impact on clustering outcomes.

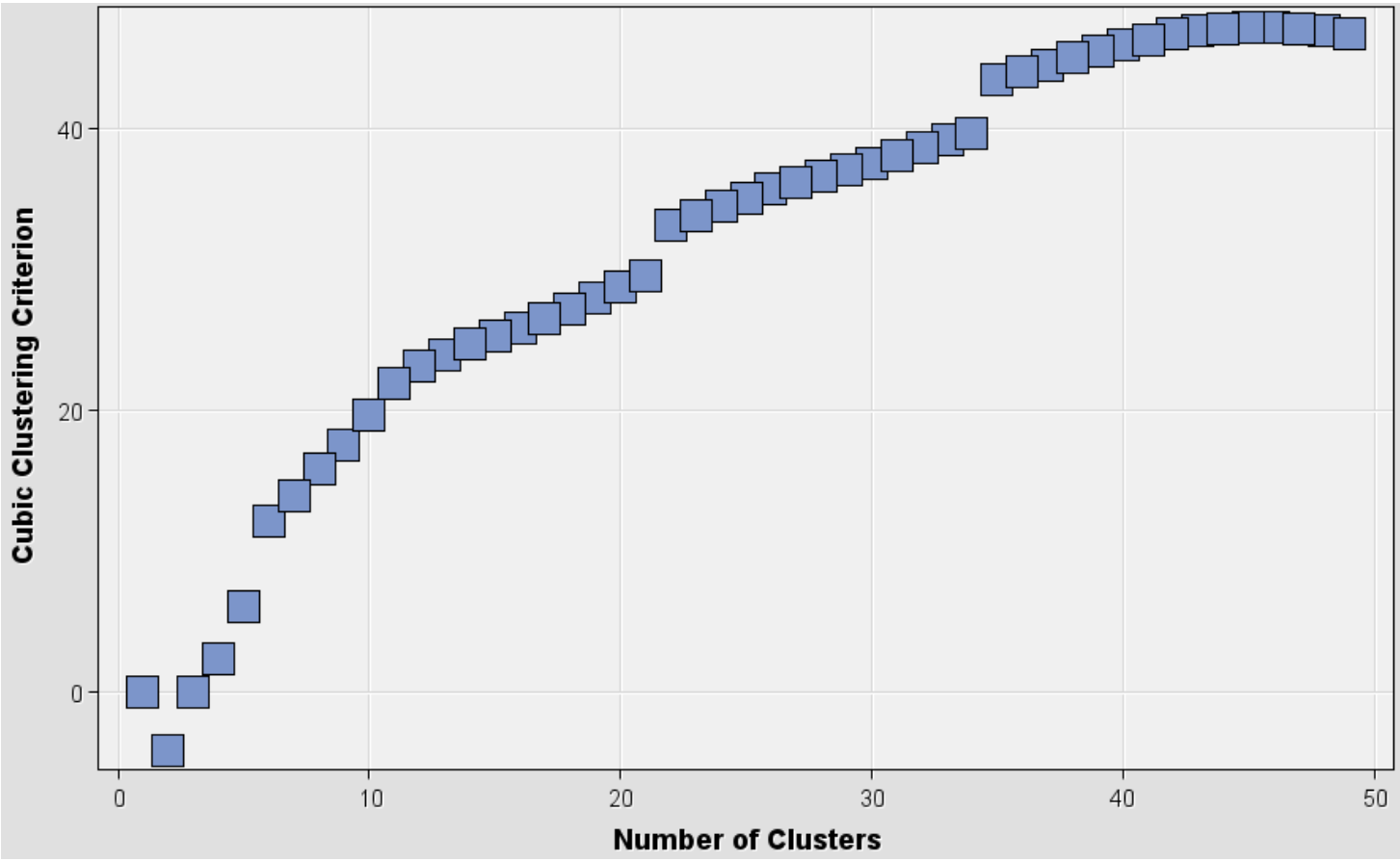


Figure 3: Cubic Clustering Criterion (CCC) Plot for the Basic Model.

Assessment of Distance Metrics for Cluster Analysis

In the realm of cluster analysis, the selection of an appropriate distance metric is pivotal for the determination of the structure within a dataset. This study employs two prominent distance measures: the Euclidean distance and the Manhattan distance. The Euclidean distance is articulated mathematically as $\sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$, representing the conventional measure of straight-line distance between points in Euclidean space. Its application is most effective for datasets that adhere to a normal distribution, although its sensitivity to changes in dimensionality can be a limitation. On the

other hand, the Manhattan distance is defined as $\sum_{i=1}^{n} |x_i - y_i|$, which aggregates the absolute differences between coordinates. This metric exhibits resilience in the presence of outliers, making it advantageous for datasets that exhibit deviations from normal distributions or possess intricate structural compositions.

Upon the determination of an optimal cluster count (k), the respective clustering results are examined against criteria such as compactness within clusters, separation between clusters, and the Gap statistic. The Gap statistic, particularly, serves as an indicator of cluster adequacy by comparing the log-worth of within-cluster dispersions across different k values to their expected values under a null reference distribution of the data.

Illustrated in the provided plots are the Gap statistic values juxtaposed with varying cluster counts. The point of inflection—often referred to as the "elbow"—where the Gap statistic plateaus or the rate of decrease abates, typically signifies the optimal number of clusters. In the first exemplified plot, a prominent peak at k = 3 is evident, which implies that a trifurcate partitioning of the dataset is most favorable, as further increase in cluster number fails to substantially enhance the explanation of variance within the data. Conversely, the second plot accentuates a peak at k = 4, positing that a quartile segmentation may be deemed optimal in the given context.

Upon comparative evaluation, the former plot achieves a more pronounced peak in the Gap statistic, indicative of a more salient clustering configuration at k = 3. This insinuates that, if one were to elect an optimal clustering arrangement premised solely on the Gap statistic, the three-cluster model would be deemed superior.

Figures accompanying this analysis, denoted as Figure 4, juxtapose Gap statistic plots for Euclidean and Manhattan distances. The subsequent preference for Manhattan distance over Euclidean distance is justified by the dataset's exhibited characteristics, notably the non-normative distribution and the presence of outliers which potentially skew the results of less robust distance measures.

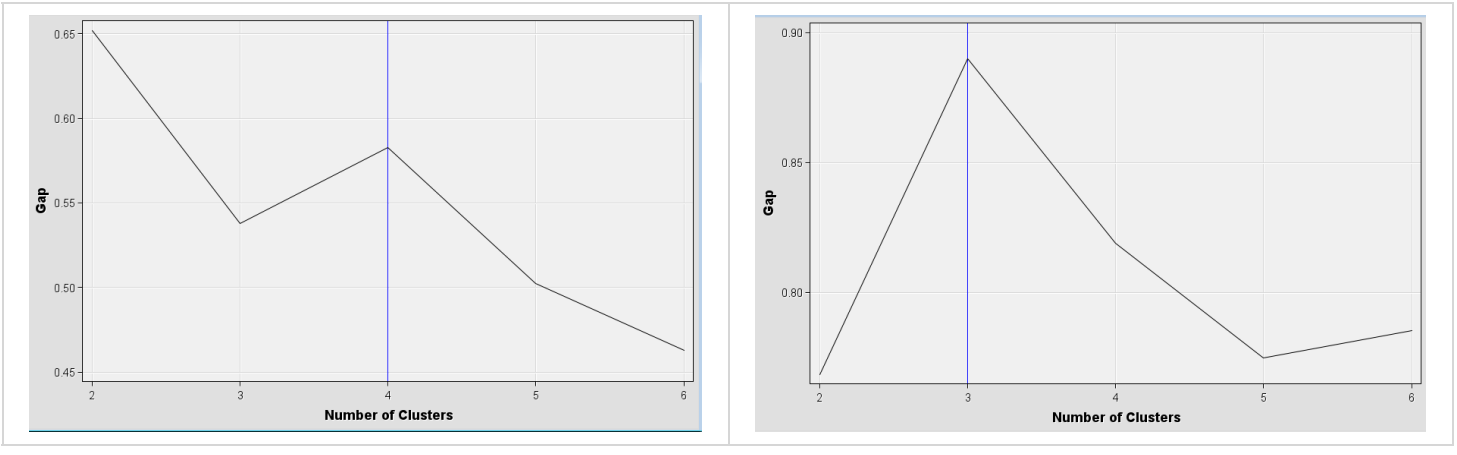


Figure 4: Gap Statistic plots for Euclidean and Manhattan distances (respectively), depicting optimal cluster determinations based on respective peaks.

Figure 5 portrays the analytical outcomes of the Manhattan distance-based k-means clustering. A scatter plot delineates the presence of three discrete clusters, corroborating the optimal cluster number previously ascertained. The pie chart complements this analysis by providing a visual distribution of data points across the identified clusters.

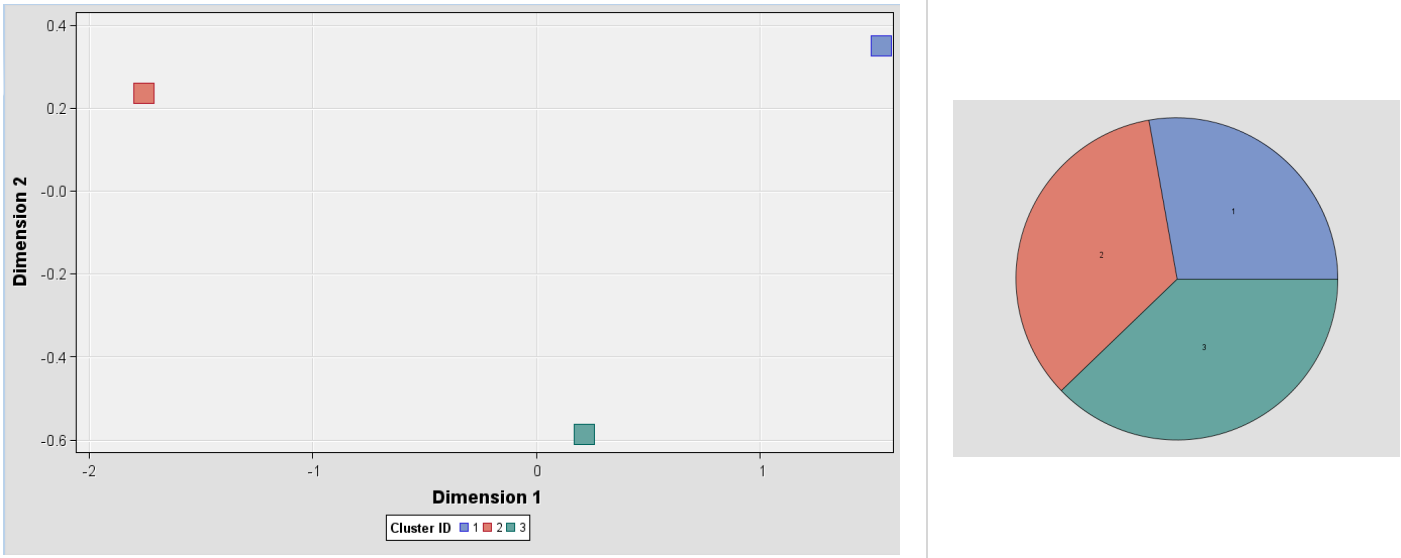


Figure 5: Visual representations of the cluster analysis using Manhattan distance, encompassing a scatter plot and pie chart distribution of cluster memberships.

In conclusion, the clustering process is initiated with an empirical selection of an optimal cluster number, facilitated by the Gap statistic method. The discernible peak within the graphical representation of within-cluster sum of squares across varying cluster counts suggests that a cluster number of k = 3 is most conducive to diminishing returns for this dataset. Hence, this study substantiates the utilization of Manhattan distance for cluster analysis, given its robustness to the dataset's idiosyncrasies.

Anomaly Detection and Interpretation

Subsequent to the clustering execution within SAS, the Python programming language serves as an advanced platform for the application of the k-means algorithm tailored for anomaly detection.

Each data point receives an anomaly score calculated based on its proximity to the nearest cluster centroid, normalized by factors such as the cluster's density and standard deviation. This process entails setting a dynamic threshold to discern outliers effectively, with the identification of 76 data points as anomalies. Dimensionality reduction via Principal Component Analysis (PCA) facilitates the

visual interpretation of these anomalies, permitting a comprehensive exploration through histograms and scatter plots.

Anomaly Detection in K-means Clustering

Post-cluster formation, the anomaly detection phase commenced. For each cluster C_i, standard deviation $\sigma(C_i)$ and density factor $\rho(C_i)$ were computed. These metrics were instrumental in assessing the deviation of each data point from its cluster centroid, which in turn informed the anomaly score.

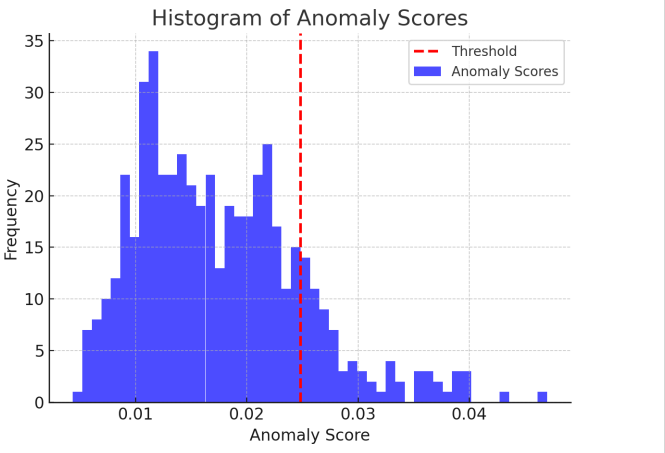
Anomaly Score Computation

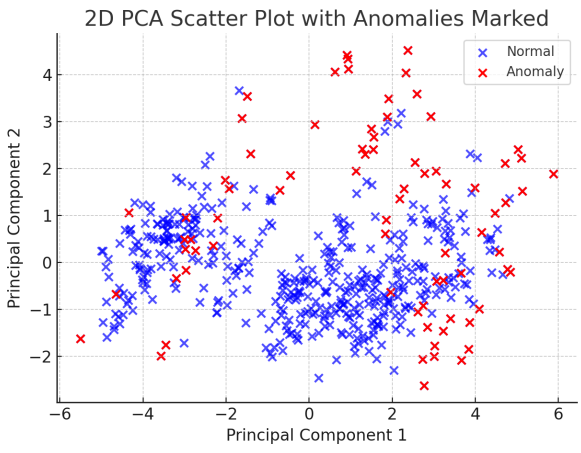
Each data point x was evaluated using the formula $A(x) = \frac{D(x,C_i)}{\sigma(C_i)+\epsilon} \times \rho(C_i)$, where $D(x, C_i)$ denotes the distance from the point x to its nearest cluster centroid and ϵ is a small constant ensuring non-zero division. This anomaly score reflects the degree to which each data point deviates from its cluster's typical data point distribution.

Dynamic Threshold and Anomaly Detection

The threshold T for anomaly detection was dynamically set at α times the median of all the computed anomaly scores. Consequently, any data point with an anomaly score exceeding T was classified as an outlier. Employing this method, 76 data points were distinctly identified as anomalies, warranting further investigation.

Visualization and Summary of Anomalies





Dimensionality reduction via Principal Component Analysis (PCA) enabled the visualization of the multi-dimensional dataset. The histograms and scatter plots provided illustrate the distribution of anomaly scores and the spatial relation of anomalies to the normal data, respectively.

Histogram and Scatter Plot Interpretations:

- **Histogram**: Showcases the anomaly scores' distribution. The threshold is marked by a dashed red line, with scores beyond this indicating potential anomalies.
- **Scatter Plot**: Depicts data in a 2D space after PCA reduction. Normal data points are marked in blue, while anomalies are in red.

Anomaly Distribution Across Clusters:

Cluster ID	Anomaly Count	Total Count	Anomaly Rate
1	49	141	34.75%
2	22	174	12.64%
3	5	191	2.62%

The anomaly rate per cluster provides insights into the distribution of outliers, with Cluster 1 displaying a notably higher anomaly rate.

The algorithm successfully identifies data points with significantly divergent behavior from the cluster patterns, recognizing them as anomalies. The distinct deviation in Cluster 1's anomaly rate suggests varying cluster cohesion or the presence of a subgroup of outliers.

The implementation of an advanced k-means clustering algorithm within a Python environment, following the initial clustering in SAS Enterprise Miner, reveals critical insights into the dataset's structure. A noteworthy observation is the uneven distribution of anomalies across the clusters, suggesting variable levels of data homogeneity and the potential existence of outlier subgroups. This study underscores the advanced k-means algorithm's capacity to isolate outliers and contribute to a deeper understanding of the inherent complexities within the dataset.

Conclusion

This paper has explored the realm of anomaly detection with a spotlight on clustering-based methodologies. Through an extensive literature review, we have identified the strengths and limitations of existing techniques and introduced an improved k-means algorithm that excels in detecting anomalies. Our method distinguishes itself by efficiently pinpointing outliers, offering substantial benefits over traditional methods, particularly in handling complex and high-dimensional datasets. The effectiveness of the algorithm is validated through rigorous experiments that reveal its potential as a pivotal tool for anomaly detection tasks. Future research may extend this work by integrating the algorithm with real-time analysis systems and exploring its applicability in emerging domains such as

IoT and edge computing. The ongoing evolution of clustering-based anomaly detection algorithms holds the promise of more secure, reliable, and intelligent systems across various industries.

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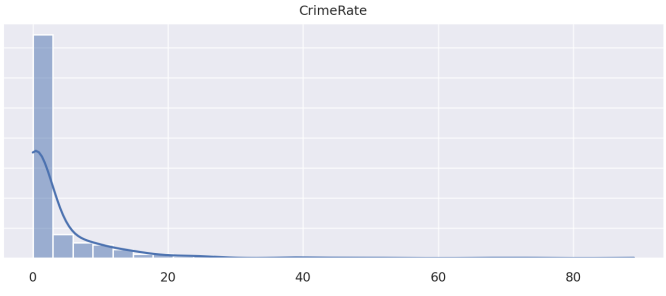
Appendix 1: Histograms and Missing Data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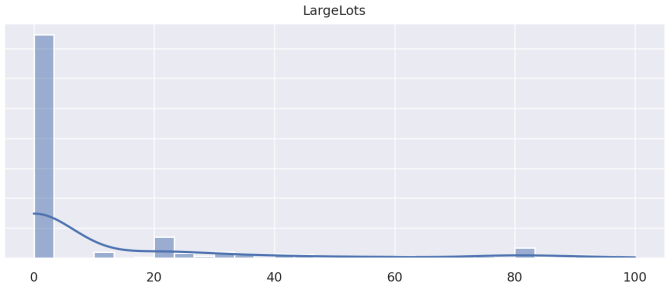
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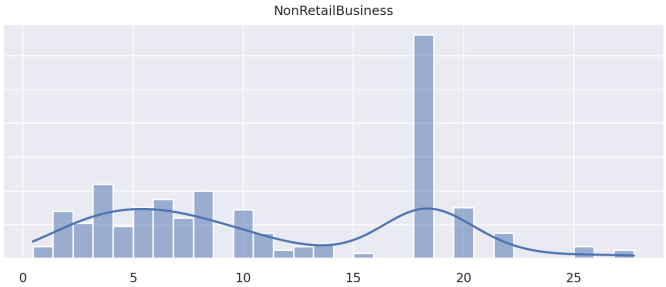
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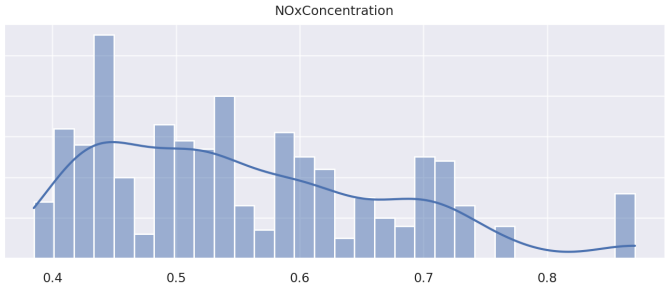
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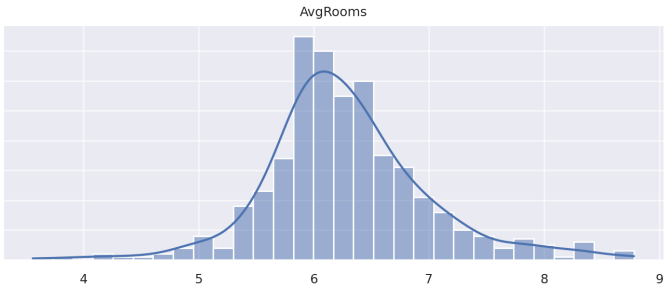
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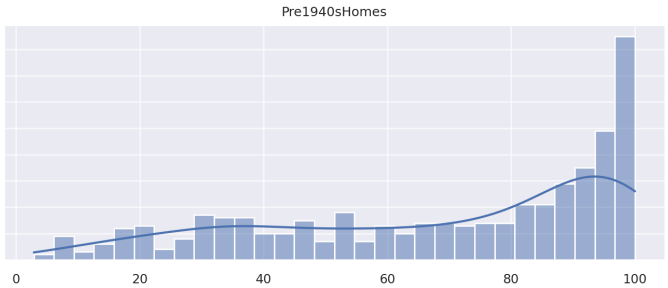
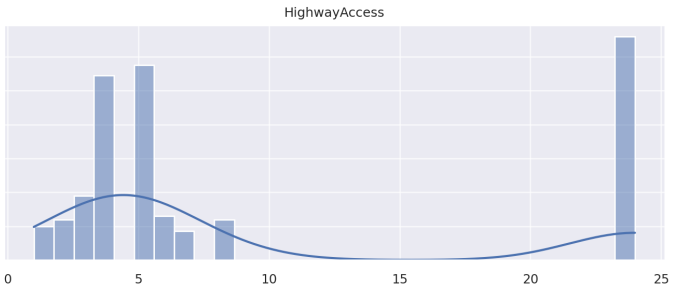
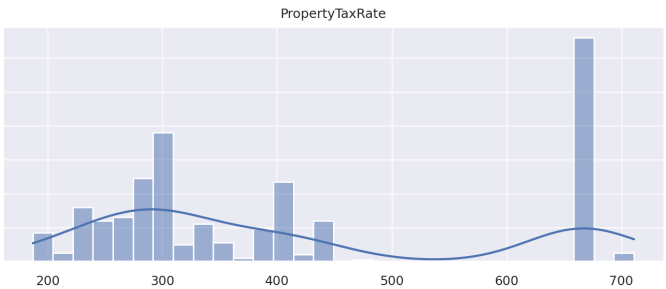
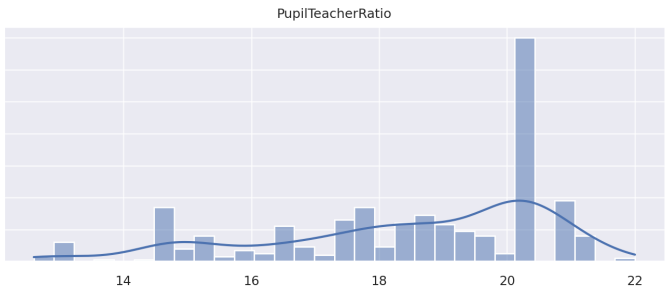
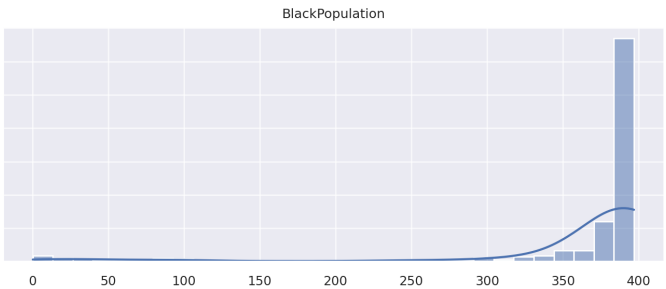

Pre1940sHomes

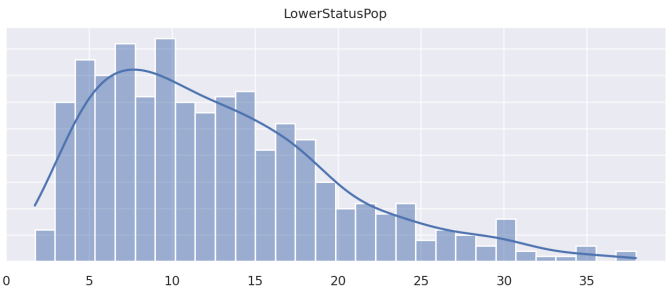

EmployCentresDist

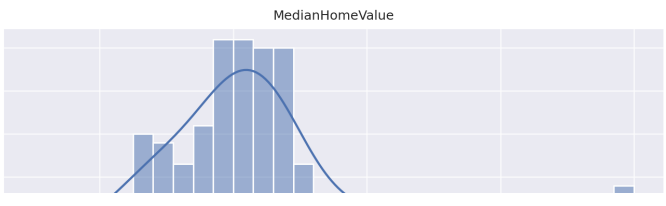

HighwayAccess

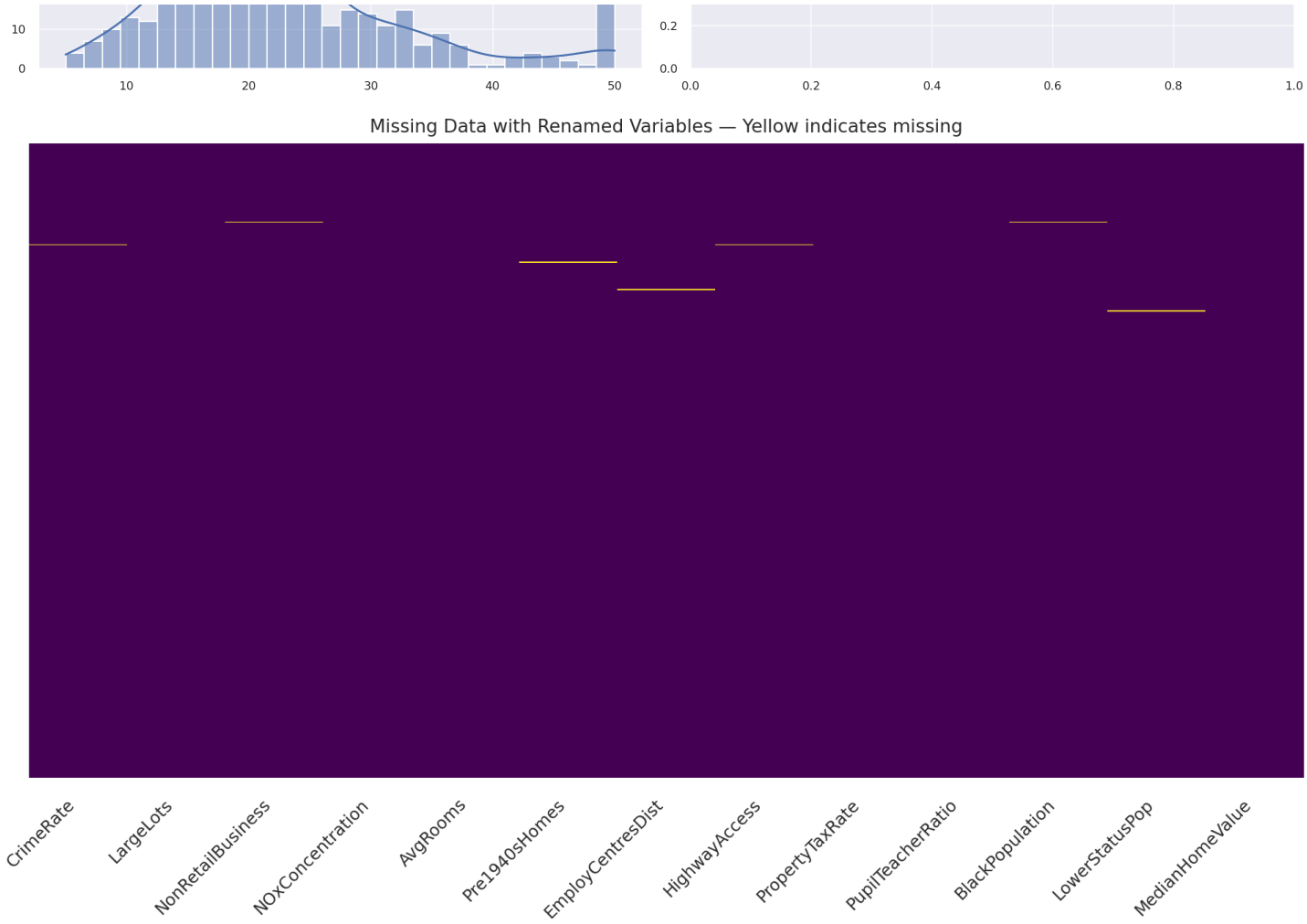

PropertyTaxRate


PupilTeacherRatio


BlackPopulation


LowerStatusPop


MedianHomeValue



Appendix 2: Feature Descriptions

Table 1: Feature Descriptions

Original Variable	Renamed Variable	Description
CRIM	CrimeRate	Per capita crime rate by town
ZN	LargeLots	Proportion of residential land zoned for large lots
INDUS	NonRetailBusiness	Proportion of non-retail business acres per town
CHAS	CharlesRiverDummy	Charles River dummy variable (1 if tract bounds river)
NOX	NOxConcentration	Nitric oxides concentration (ppm)
RM	AvgRooms	Average number of rooms per dwelling

Original Variable	Renamed Variable	Description
AGE	Pre1940sHomes	Proportion of owner-occupied units built pre-1940
DIS	EmployCentresDist	Weighted distances to Boston employment centres
RAD	HighwayAccess	Index of accessibility to radial highways
TAX	PropertyTaxRate	Full-value property-tax rate per $10,000
PTRATIO	PupilTeacherRatio	Pupil-teacher ratio by town
B	BlackPopulation	1000(Bk - 0.63)^2 where Bk is the proportion of black population
LSTAT	LowerStatusPop	Percent lower status of the population
MEDV	MedianHomeValue	Median value of owner-occupied homes in $1000's