Lab Machine Learning for Data Science

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Freie Universität Berlin

FREIE UNIVERSITÄT BERLIN

Project 1: Unsupervised Machine Learning

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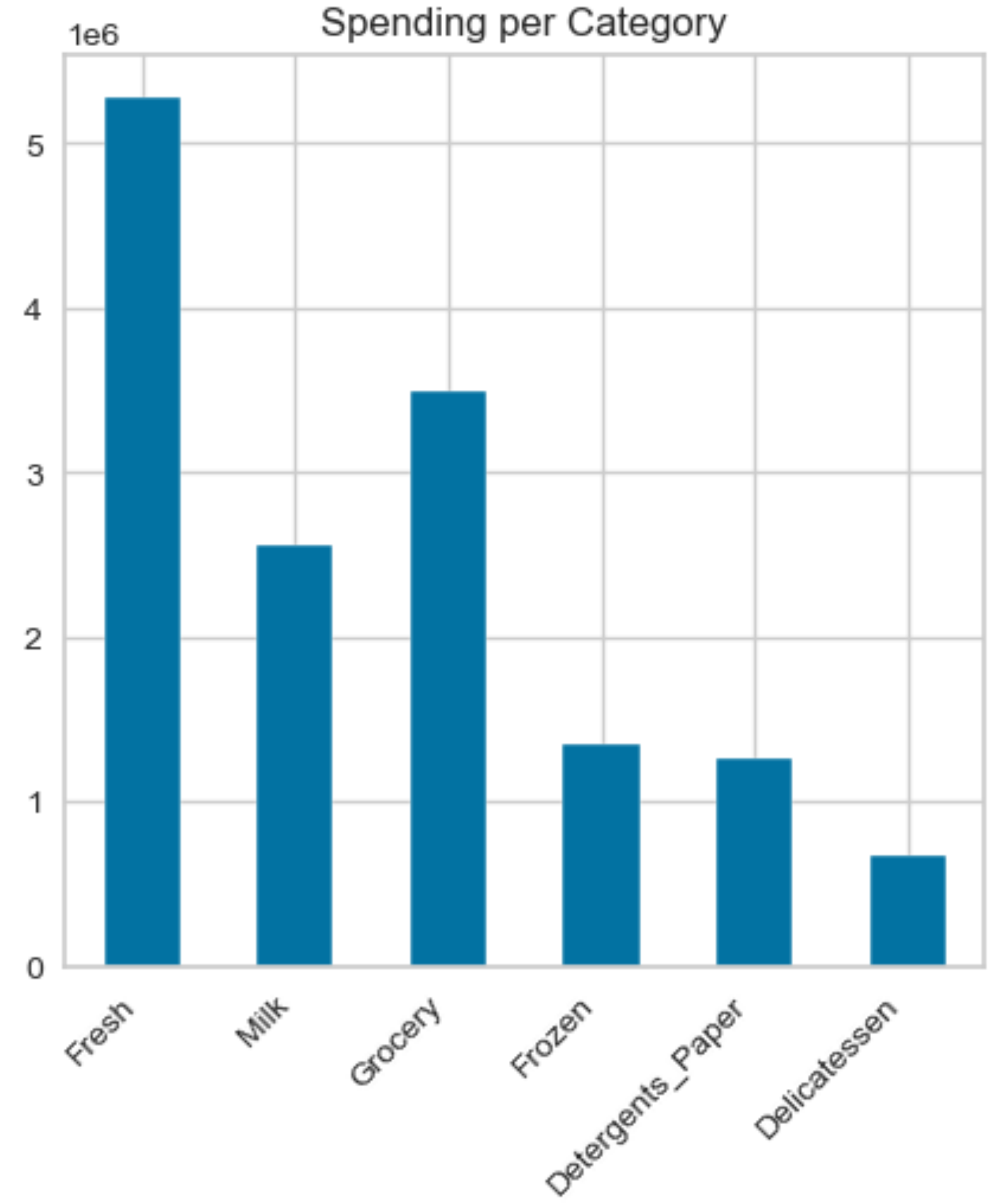
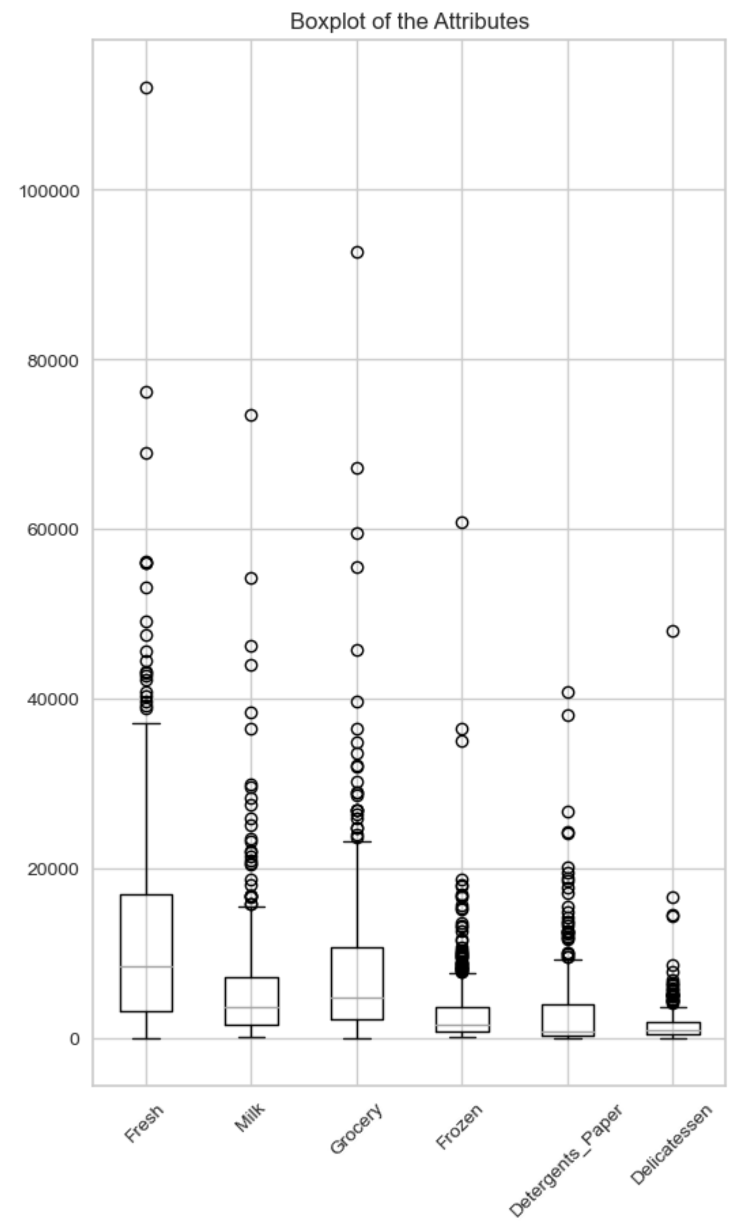
Project Goals

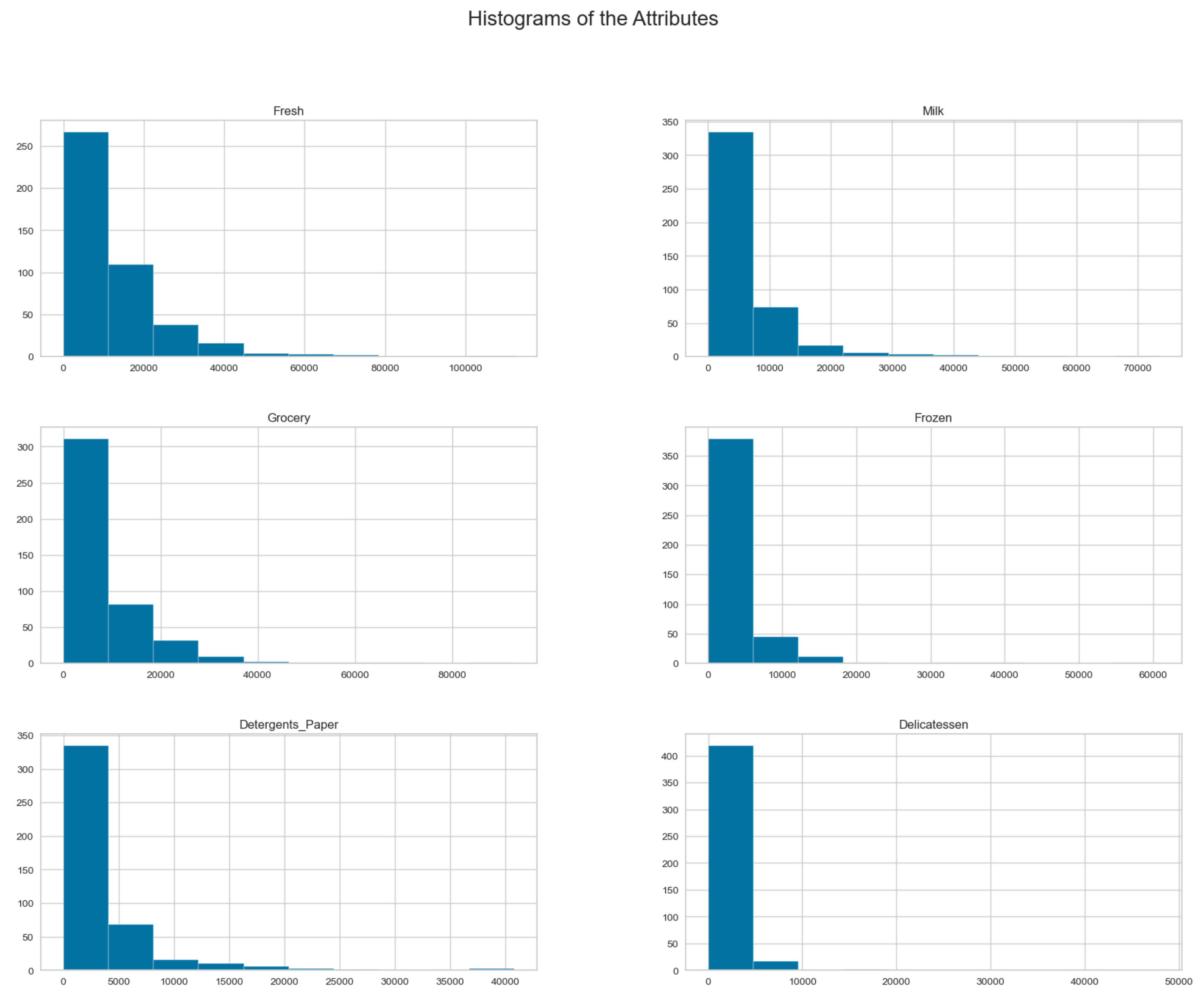
- UCI Wholesale customers dataset: annual spending on different product categories by wholesale customers located in Portugal
- → Identify instances with anomalous spending behaviour
- → Identify clusters of similarly behaving wholesale customers. In particular, we would like to leverage unsupervised ML techniques to identify anomalies and clusters.

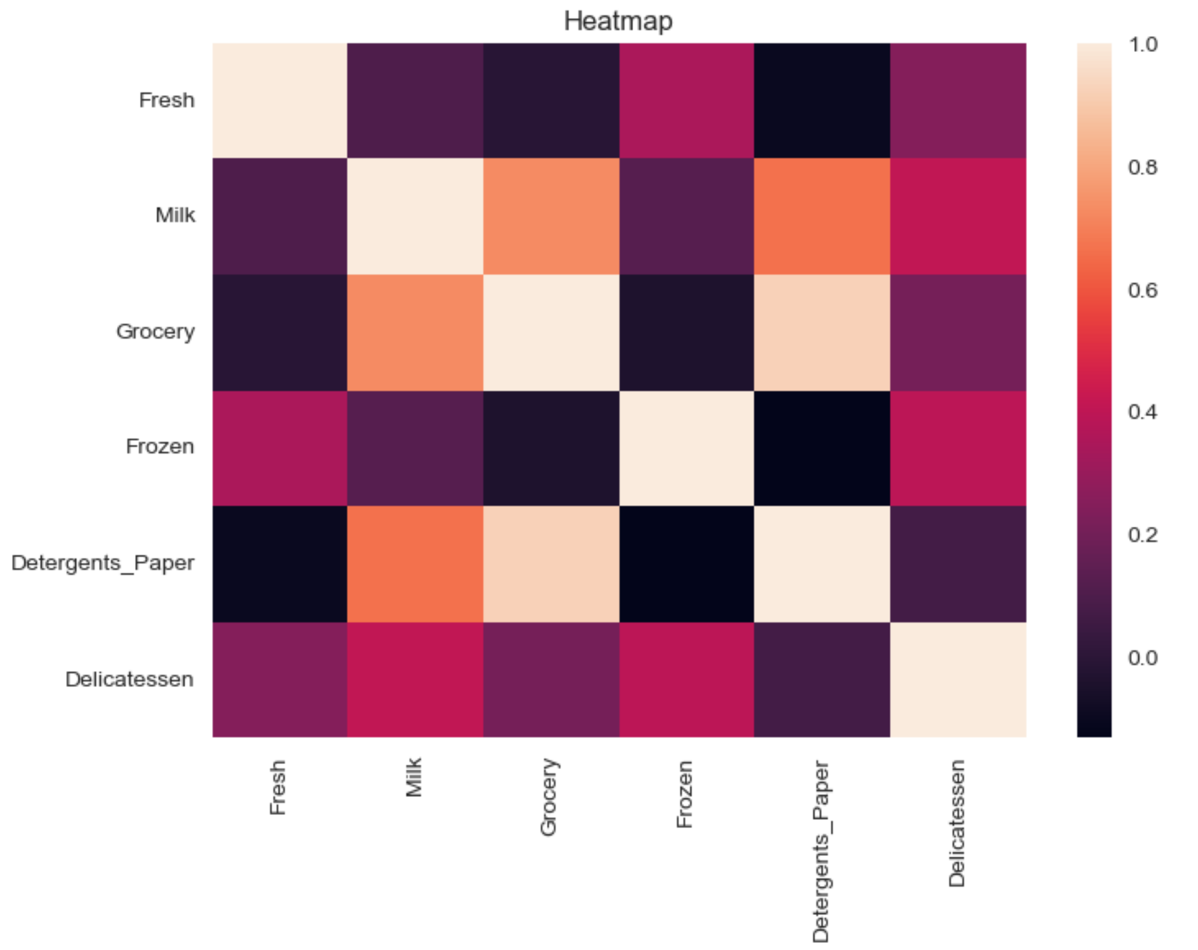
1. Initial Data Analysis and Preprocessing

- The distributions are heavy tailed → apply the log function, so that the distribution gets compressed for large values and expanded for small values

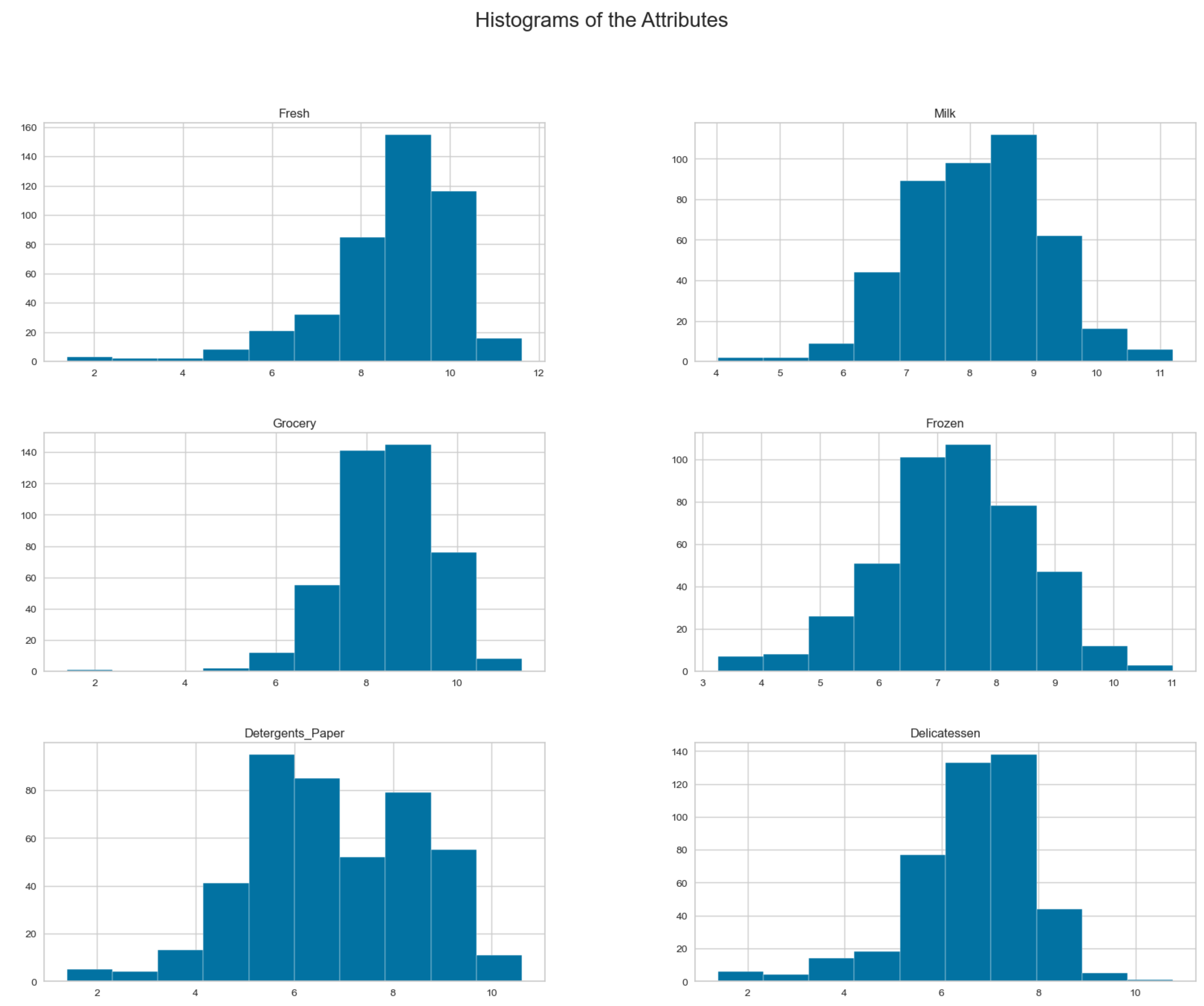


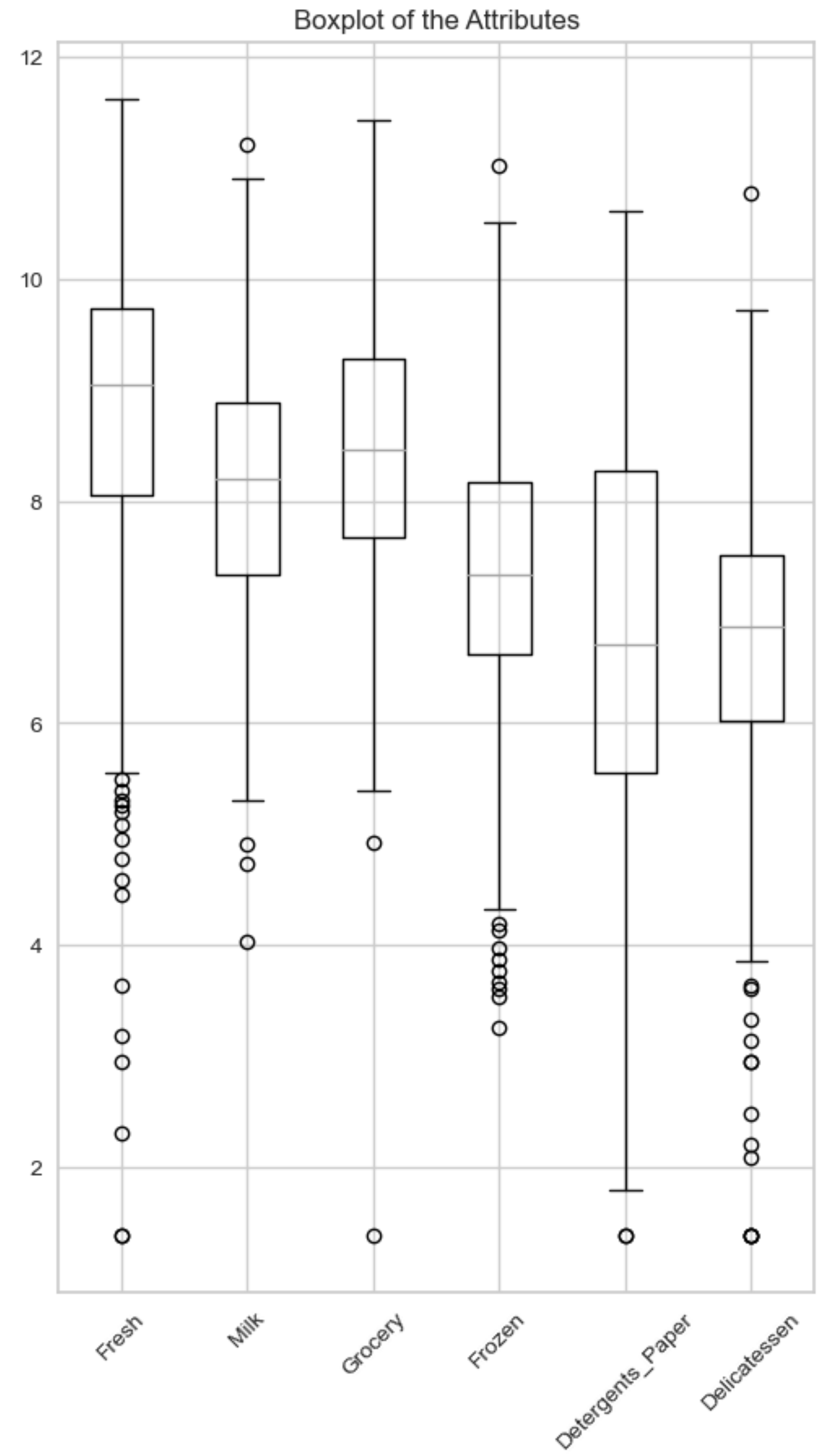






- → More normally distributed attributes
- → Few high spendings possess extreme values





2. Detecting Anomalies

2.1. Hard-Min Score

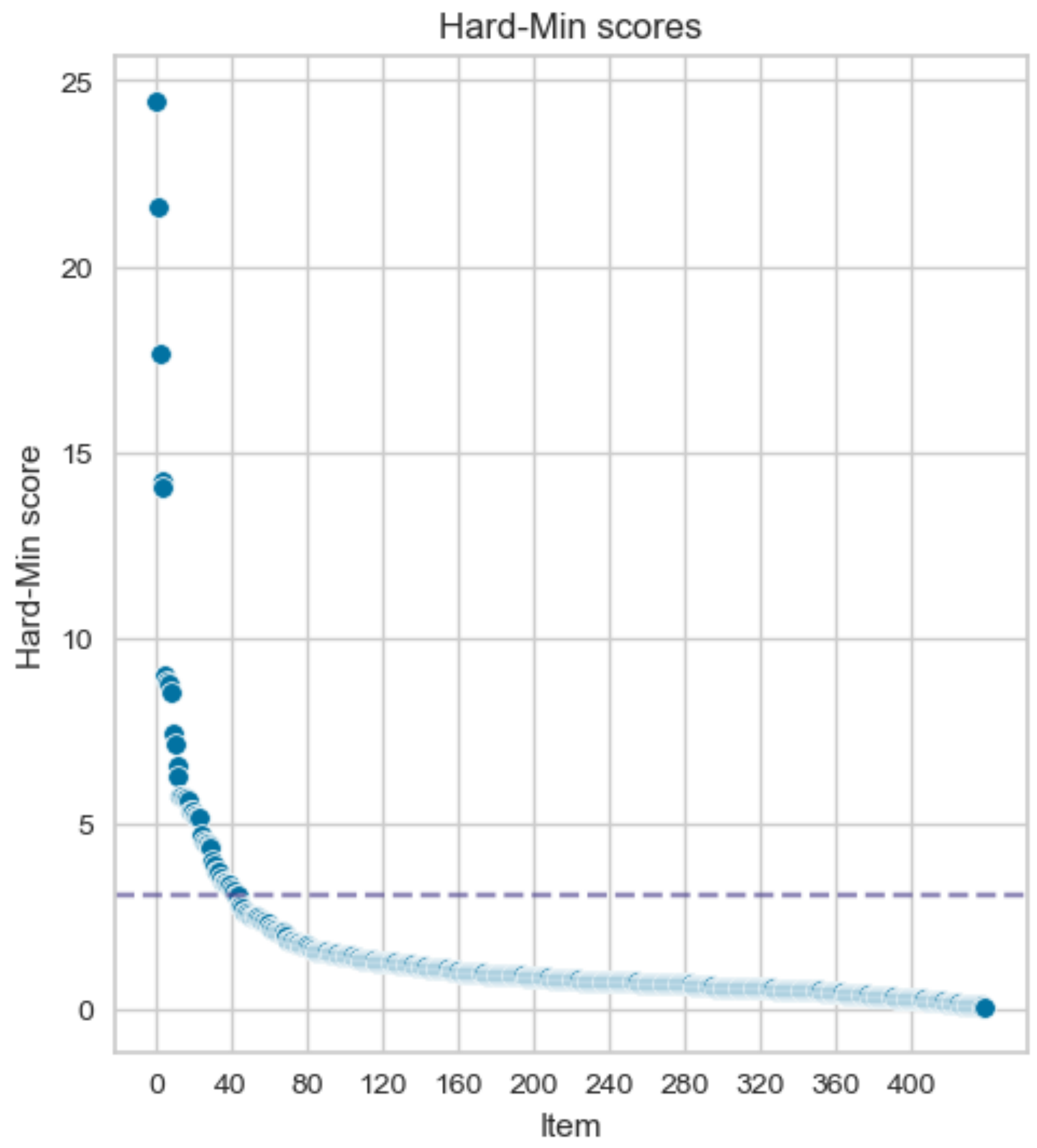
Creating Artificial Ground Truth

- **Hard-Min**: nearest neighbour distance per instance as outlier score
- For a more robust outlier score → apply **bootstrapping** with replacement, compute Hard-Min Scores for each sample.
- Average over the scores per sample → 440 x 10000 measurements
- Hyperparameters:
    - OUTLIERS_FRAC = 0.1 → based on the elbow of the Hard-Min score plot
    - N_BOOTSTRAP = 10000 → as many as computationally reasonable

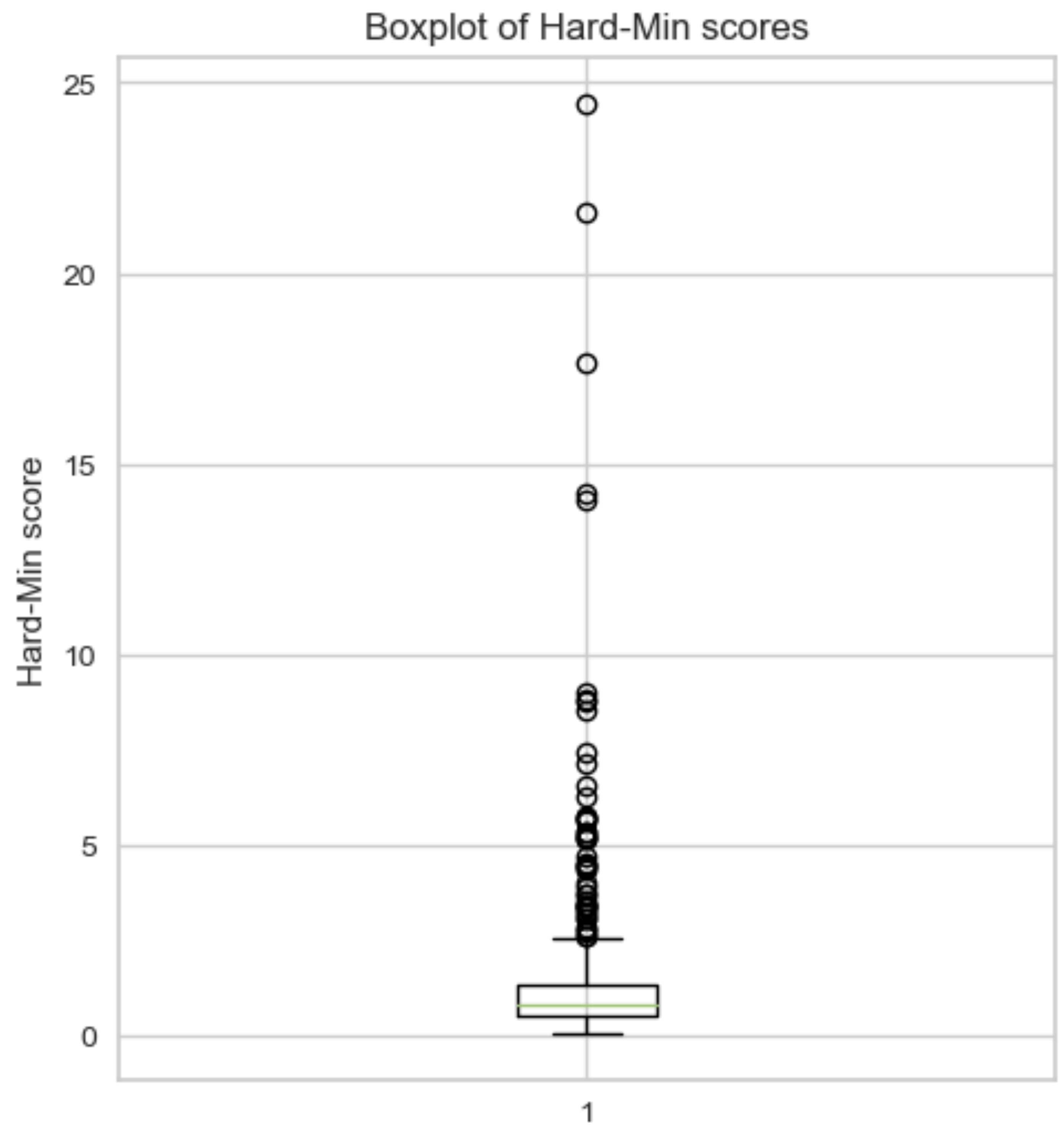
2.1. Hard-Min Score

Outliers' Fraction Determination

- 44 outliers with Hard-Min score above 3



- 51 extreme values in the Boxplot



2.1. Hard-Min Score

Evaluation: Biasedness

- → Spearman's ranking correlation
- → Accuracy of classifying the same set of outliers

```
Accuracy: 0.95%
Spearman corr.: 0.97
Spearman corr. on the fraction of outliers: 0.31
Spearman corr. on the top five outliers: 0.9
```

2.2. Soft-Min Score

Measure outlierness based on multiple neighbours

- **Soft-Min** = related to log-likelihood predicted by a kernel density estimator of the rest of the data
- **γ**: the inverse of the bandwidth or variance of the used Gaussian distributions → small γ leads to more robust estimates, but with the cost of introducing bias
- The Hard-Min and Soft-Min score distributions are similar, but they “operate” on different scales. For the Soft-Min score these scale change with change tue to the 1/gamma factor
- → makes the comparison challenging

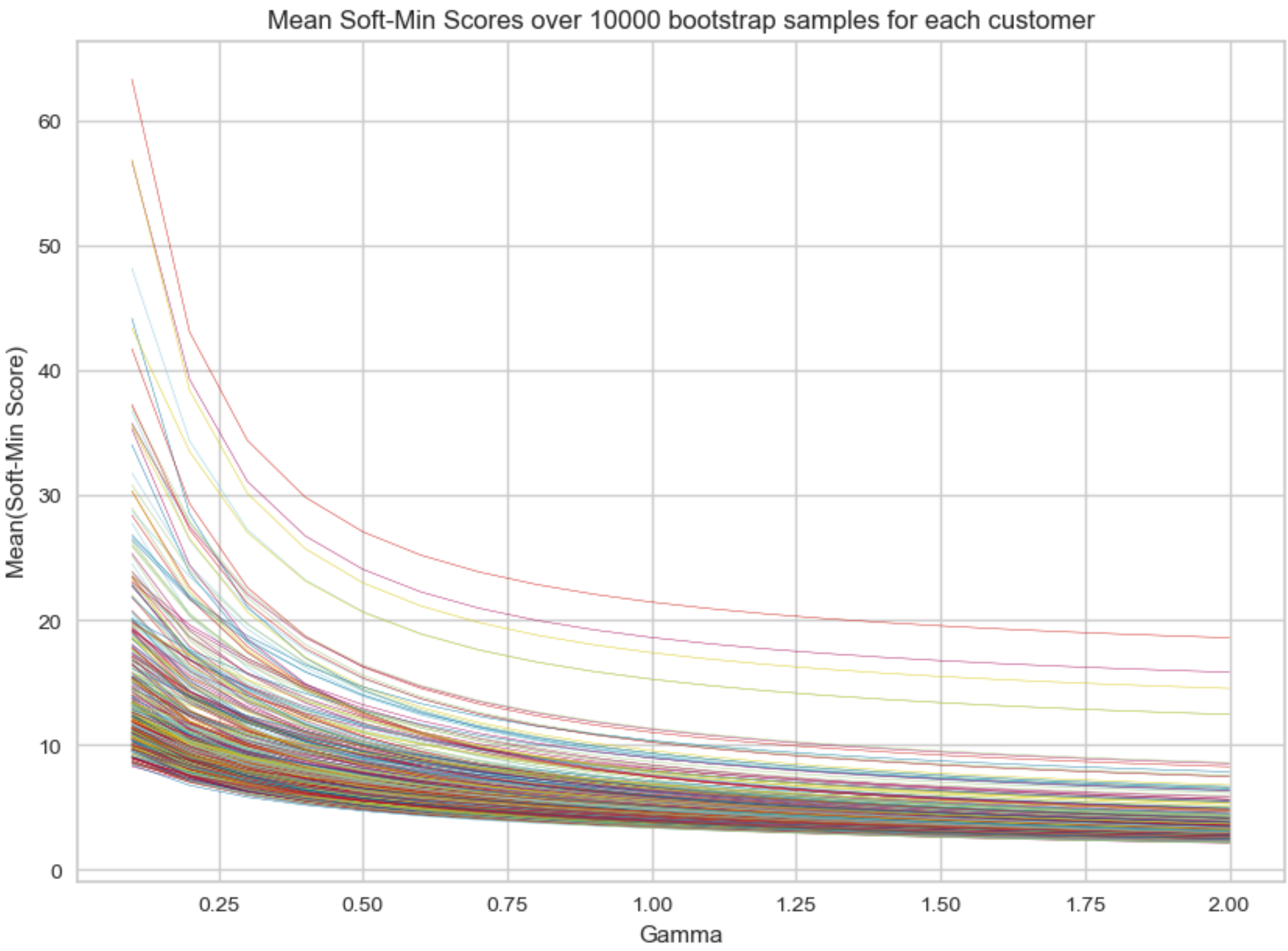
2.2. Soft-Min Score

Gamma tuning

- Apply **bootstrapping** with replacement and compute Soft-Min Scores of 20 γ values in the range [0.1, 20) for each sample.
- Average over the Soft-Min scores per sample → 440 x 10000 x 20 measurements

2.2. Soft-Min Score

Evaluation: Between Instance Variance

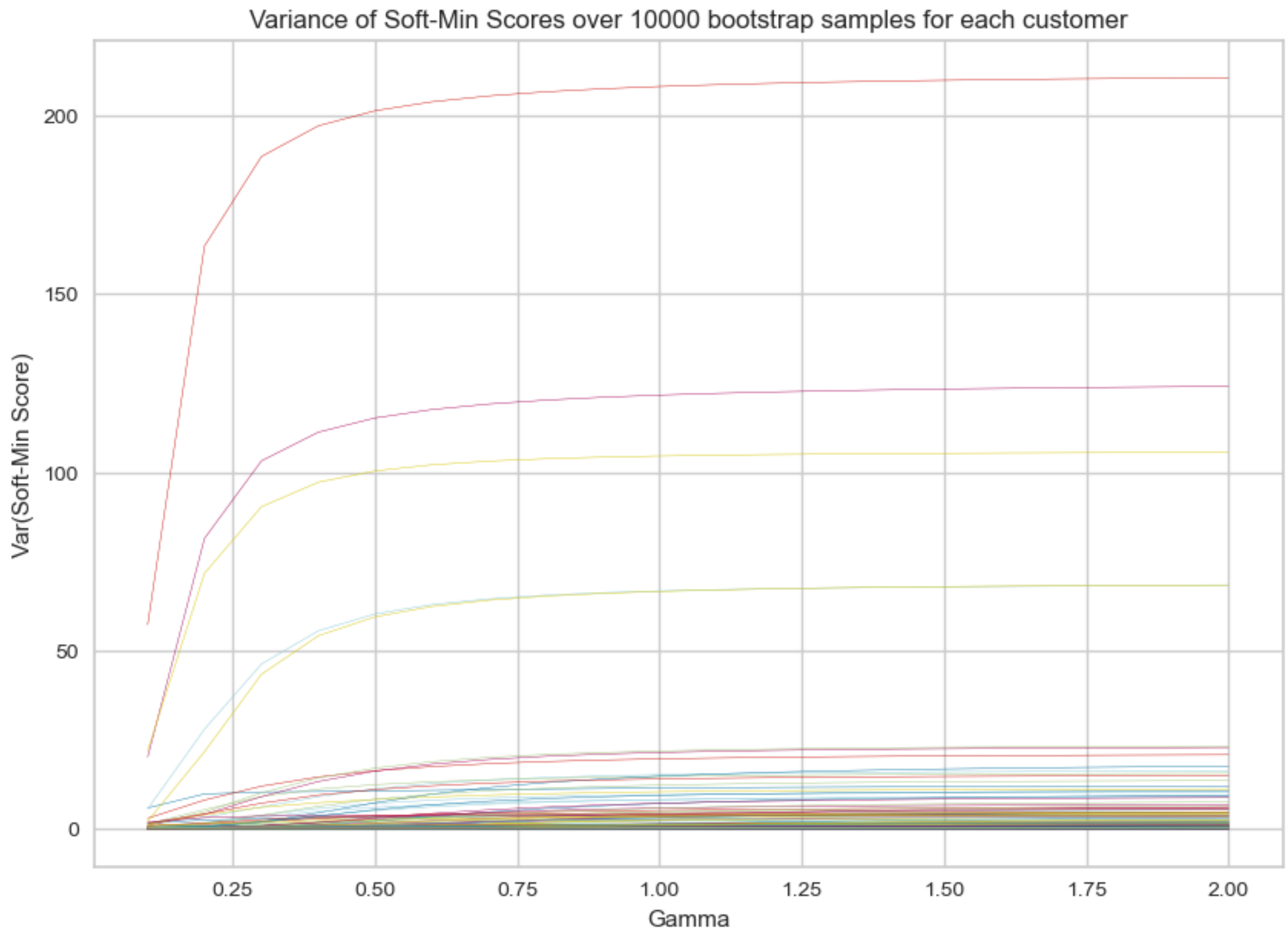


- Soft-Min scores reduce with increasing γ values
- The ranking appears to not change much
- **→ Not a good measure for discriminating ability**

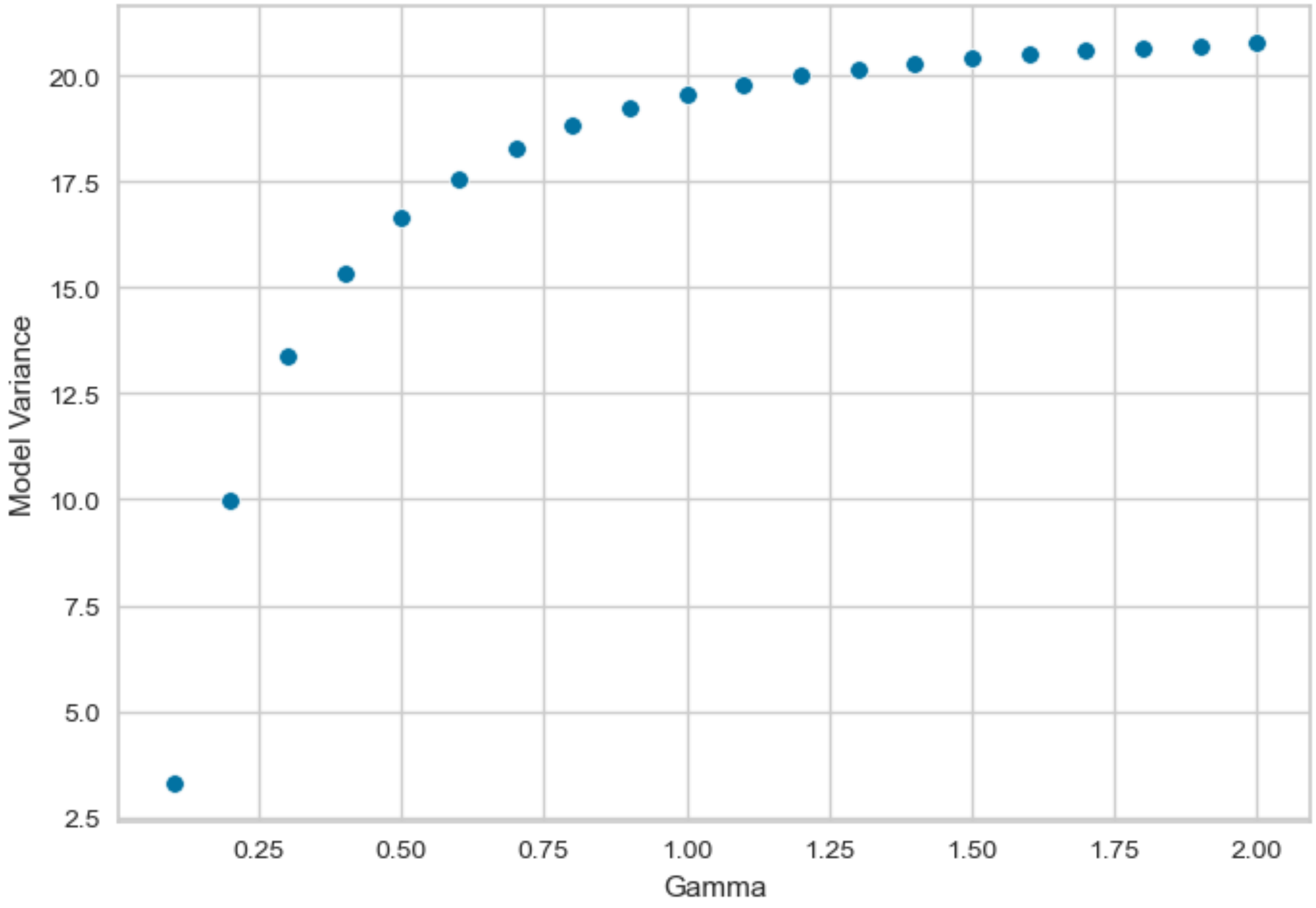
2.2. Soft-Min Score

Evaluation: Spread/Within Instance Variance

- The variance of the model increases with increasing γ values



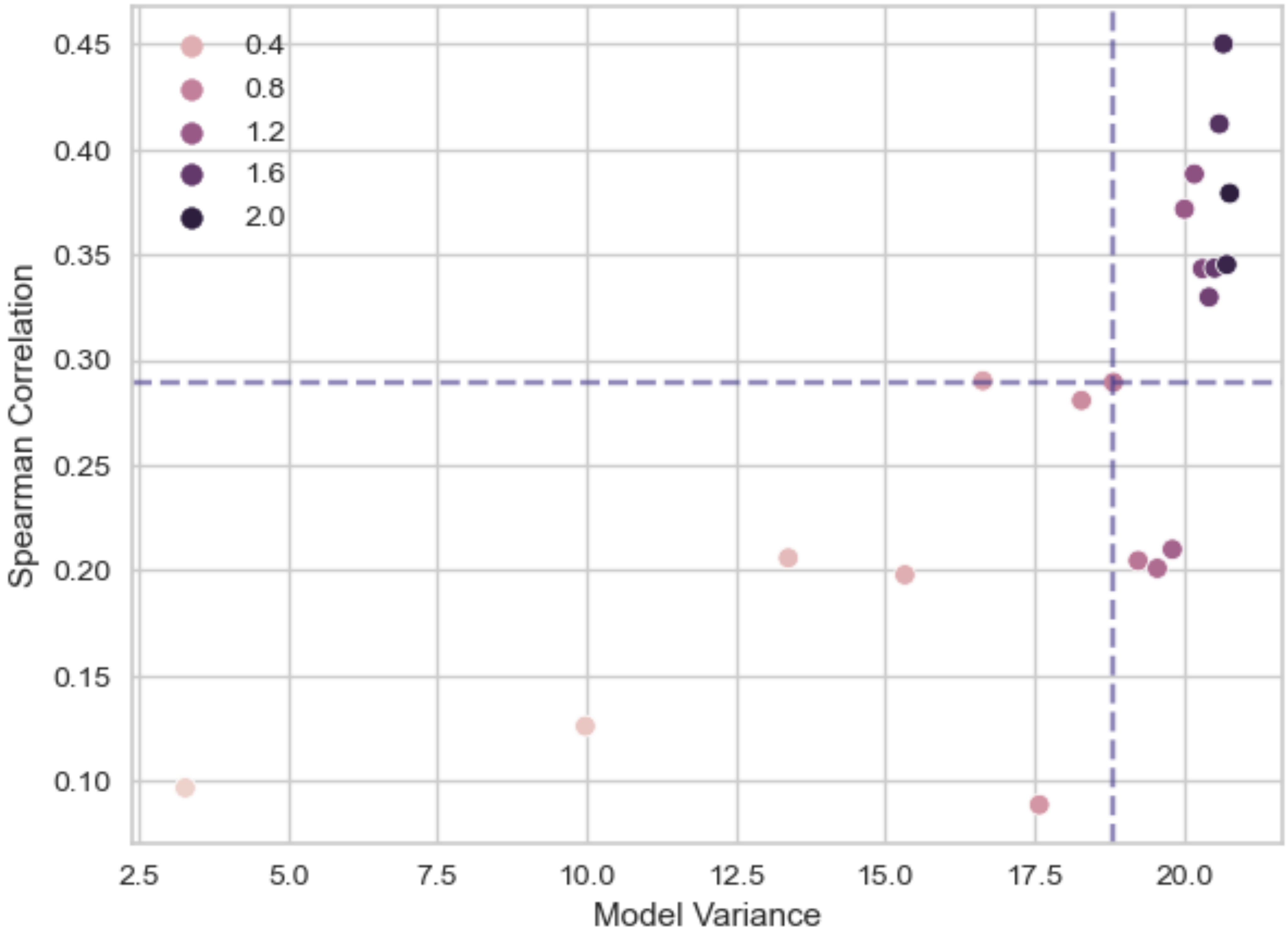
- Average over the variance of the outliers to use as evaluation metric

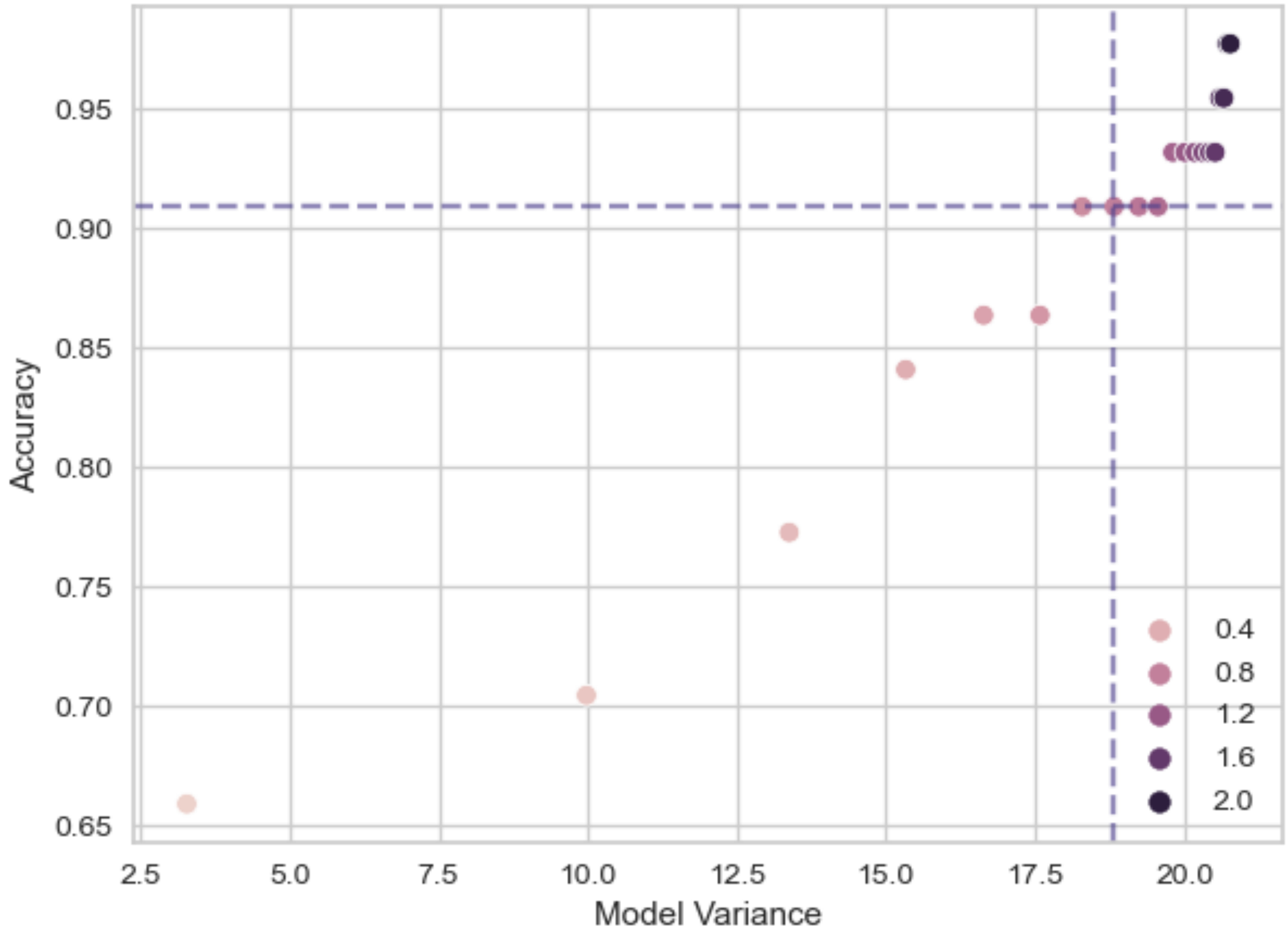


2.2. Soft-Min Score

Gamma choice: γ = 0.8

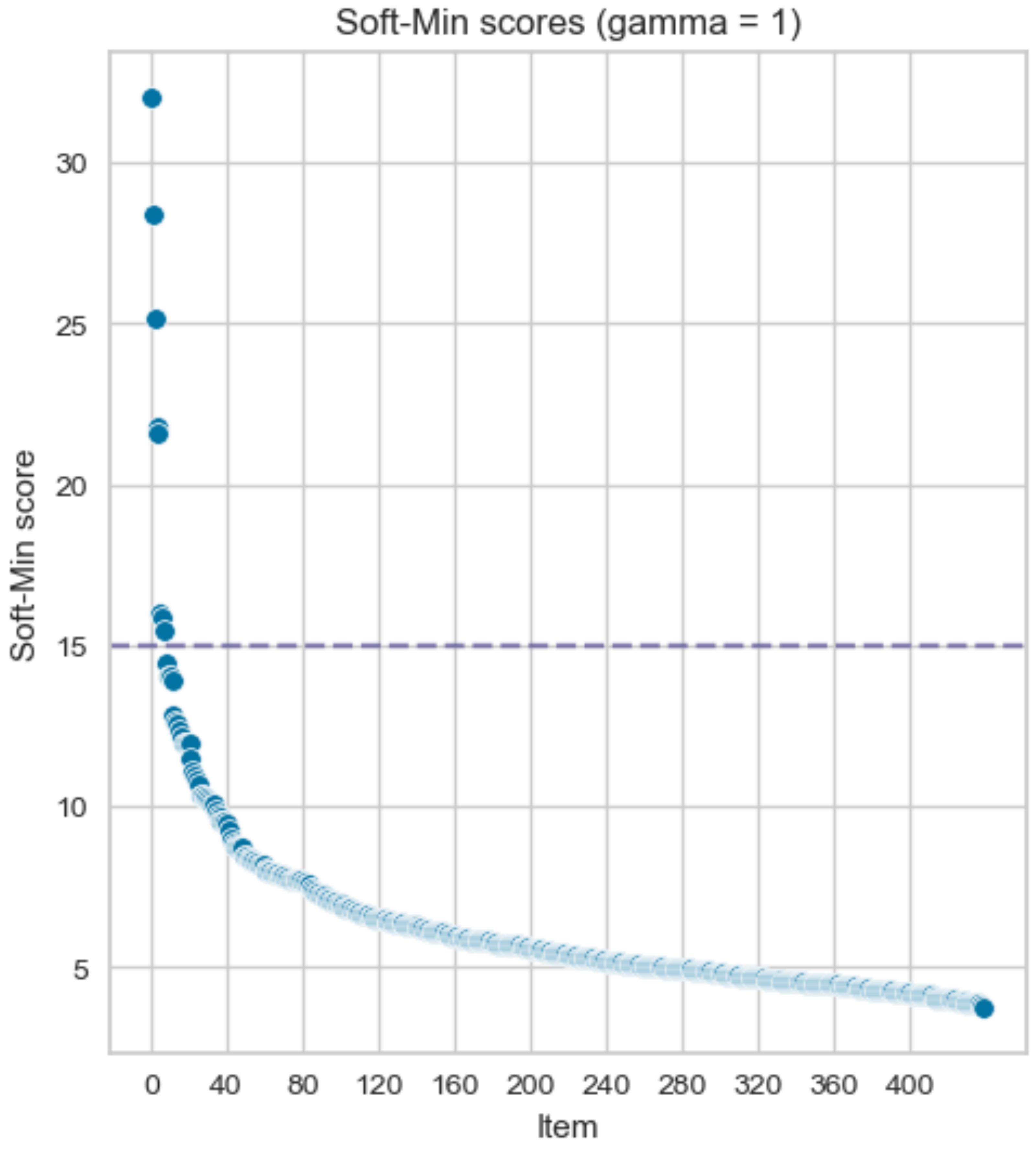
```
Accuracy: 0.91%
Spearman corr.: 0.88
Spearman corr. on the fraction of outliers: 0.41
Spearman corr. on the top five outliers: 0.9
```

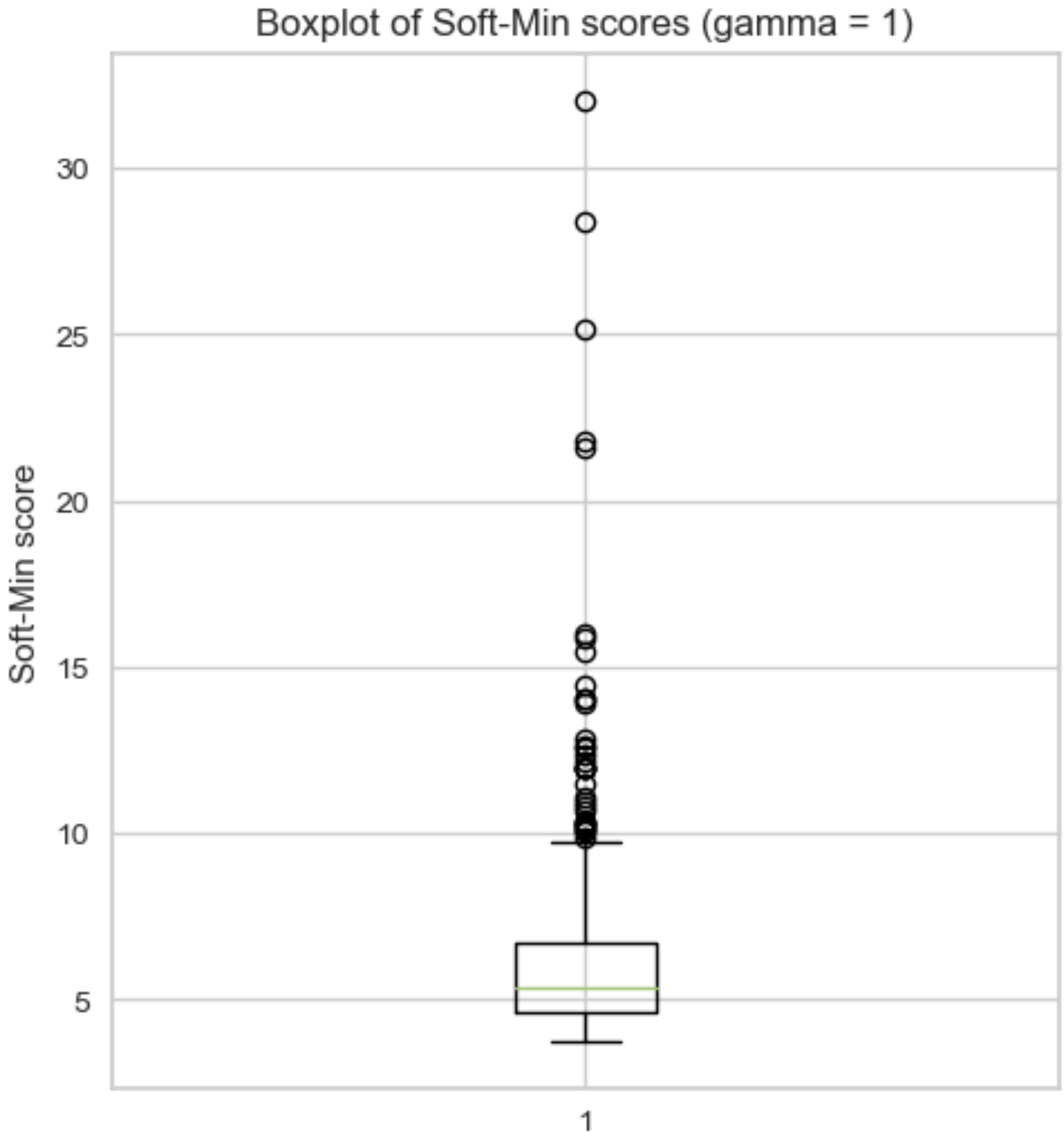




2.5. Outlier Selection

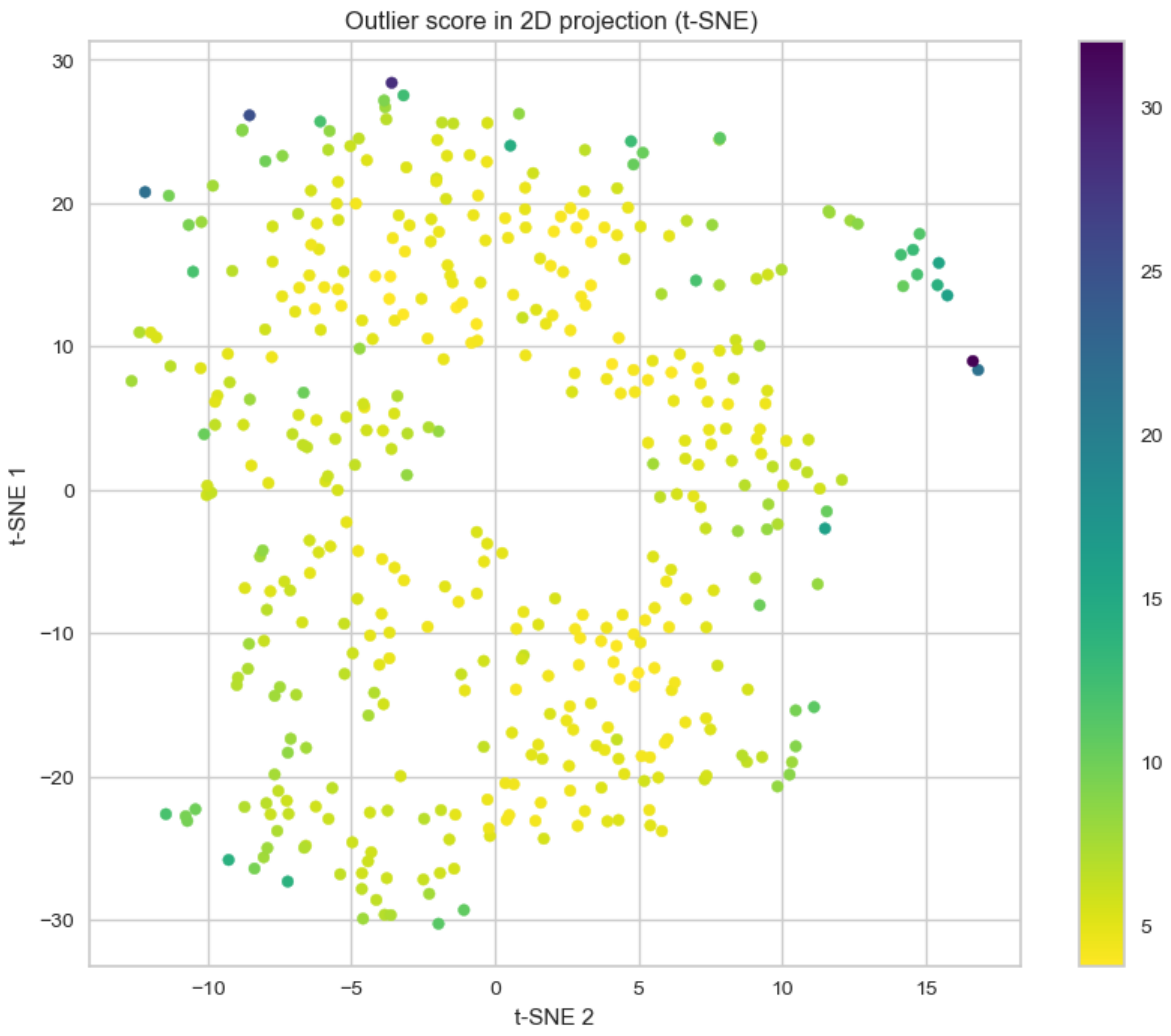
```
5 outliers above 20
8 outliers above 15
35 outliers above 9.71
```

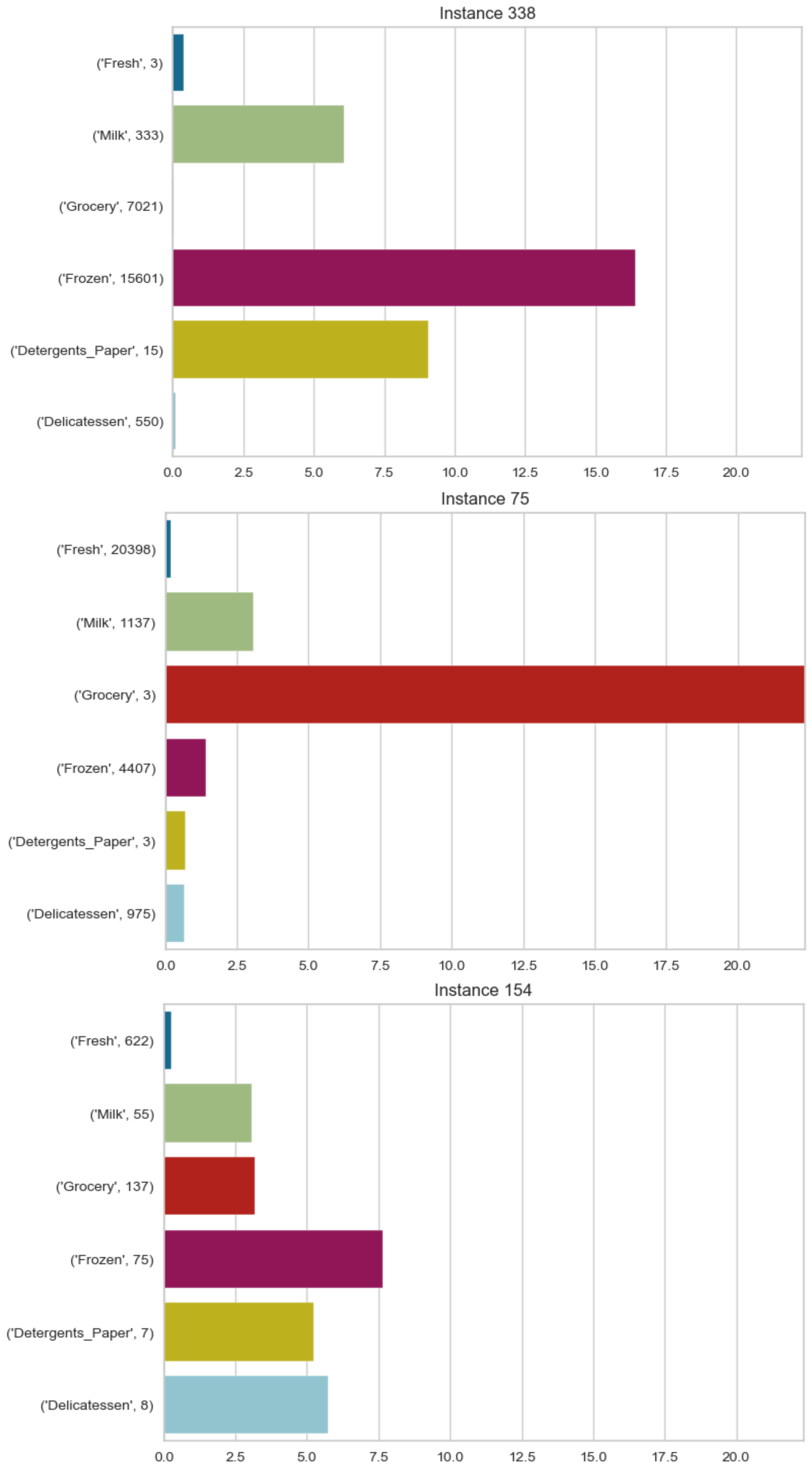




3. Explaining Anomalies

3.1. Layer-wise relevance propagation





	Fresh	Milk	Grocery	Frozen	Detergents_Paper	Delicatessen
mean	12000	5796	7951	3072	2881	1525

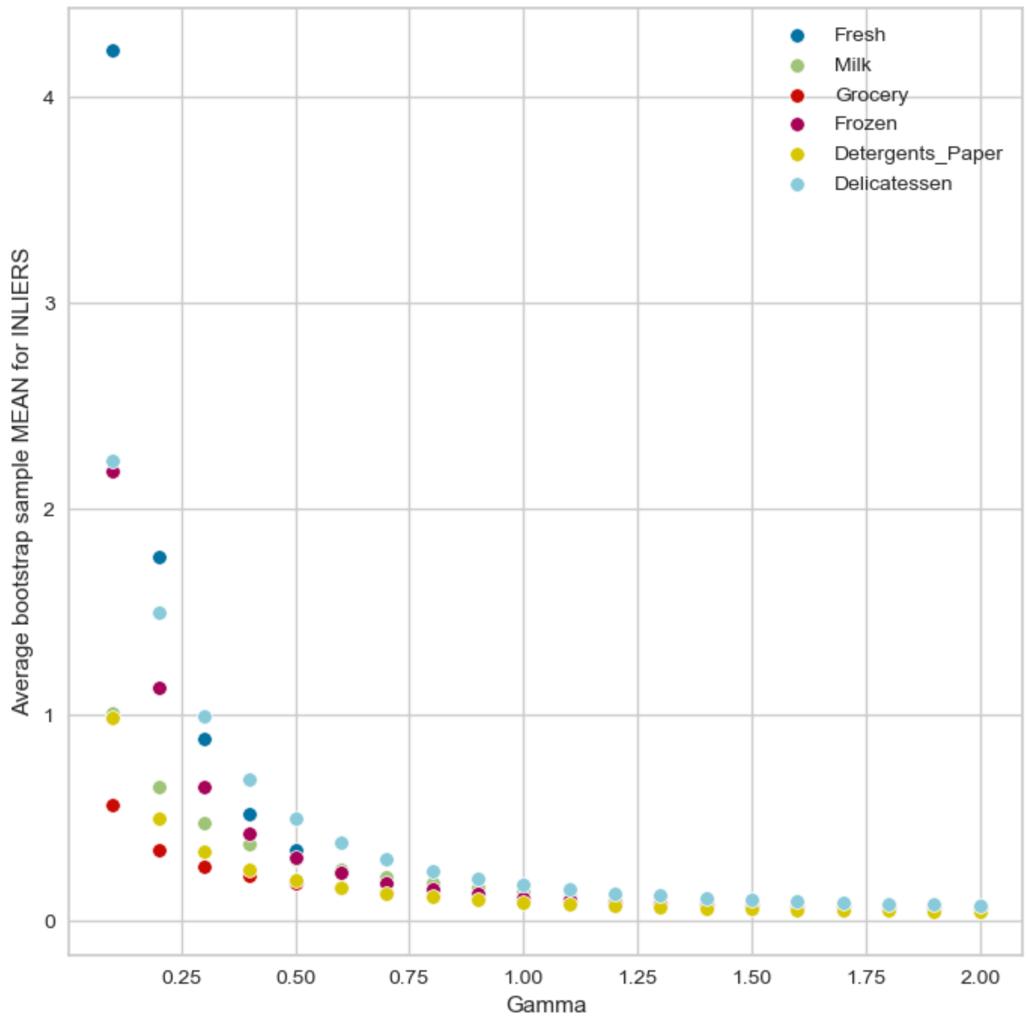
	Fresh	Milk	Grocery	Frozen	Detergents_Paper	Delicatessen
338	3	333	7021	15601	15	550
75	20398	1137	3	4407	3	975
154	622	55	137	75	7	8

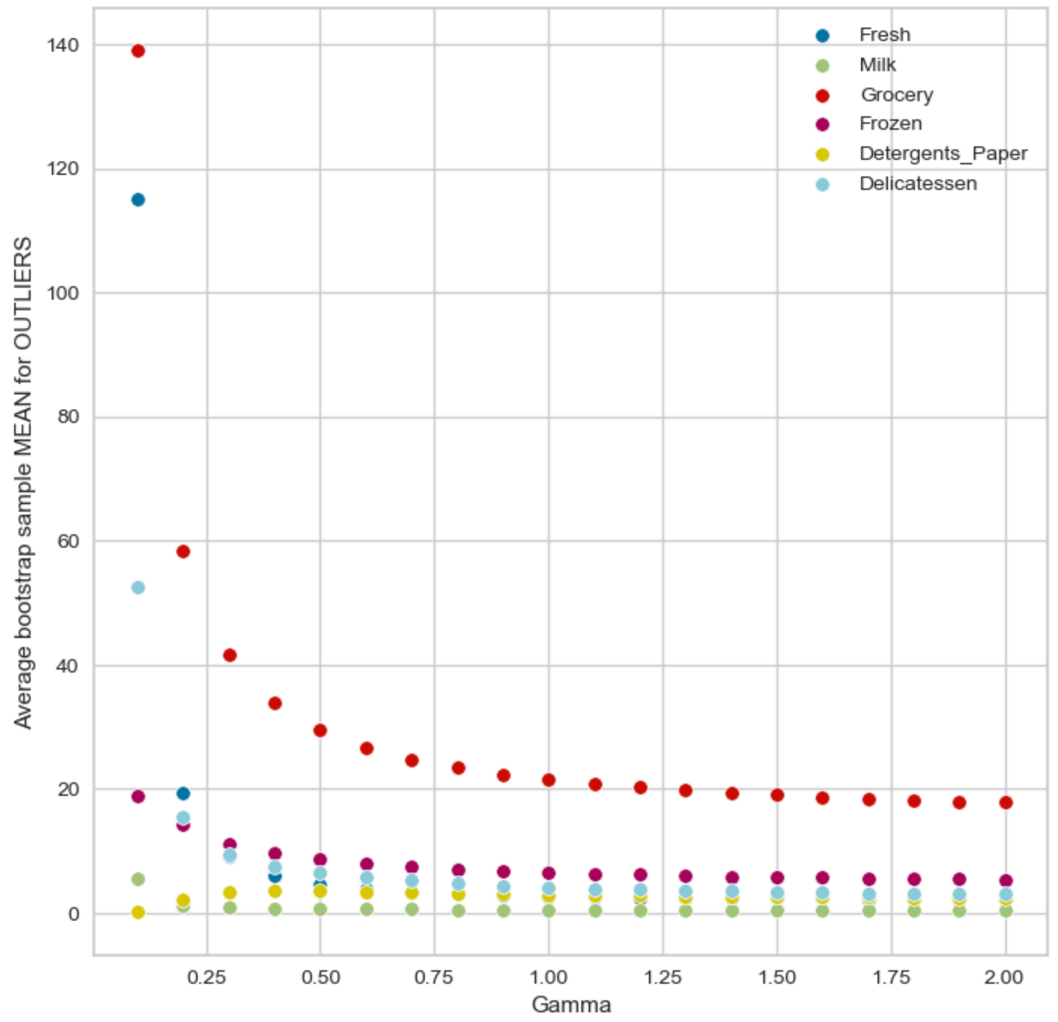
3.2. Robustness of the explanations

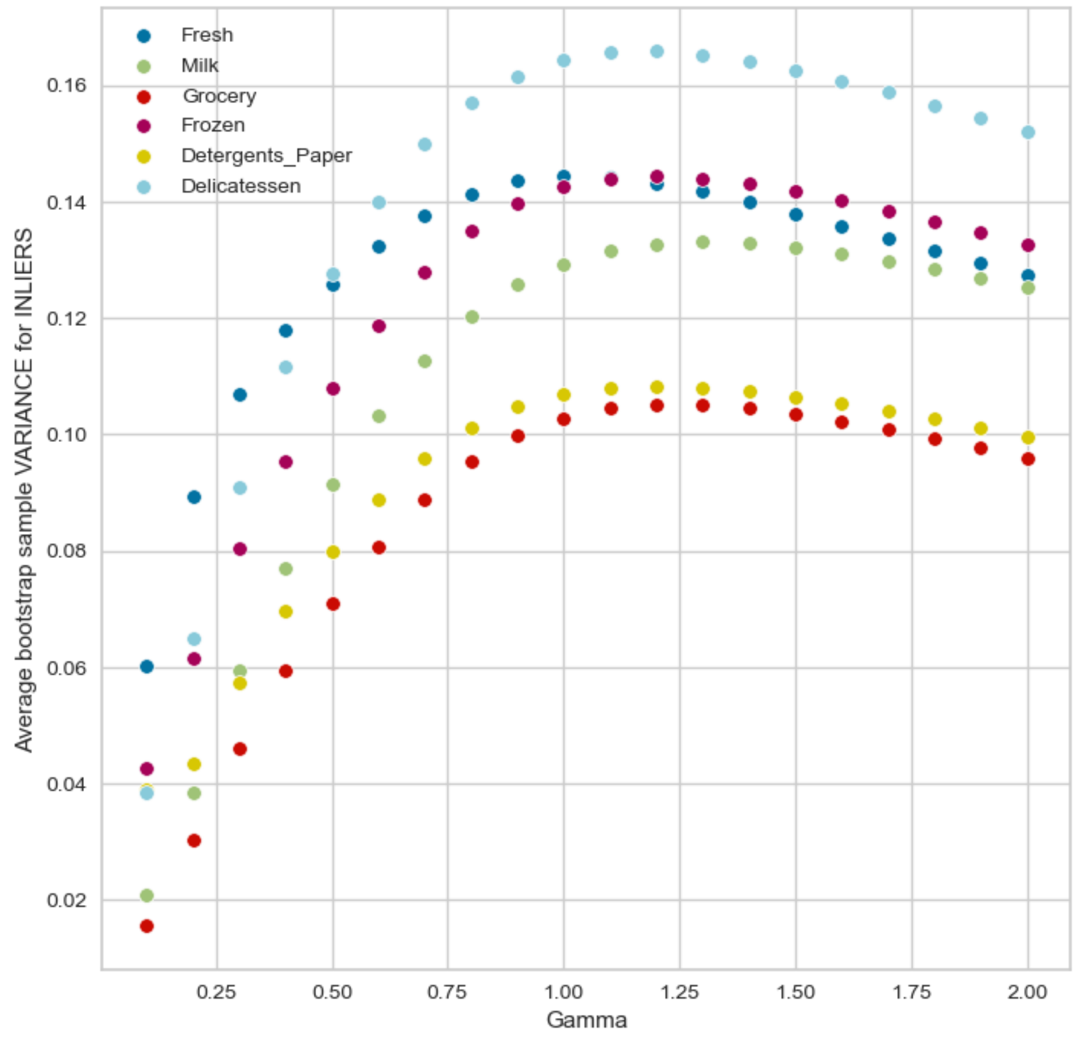
- Bootstrapping with replacement

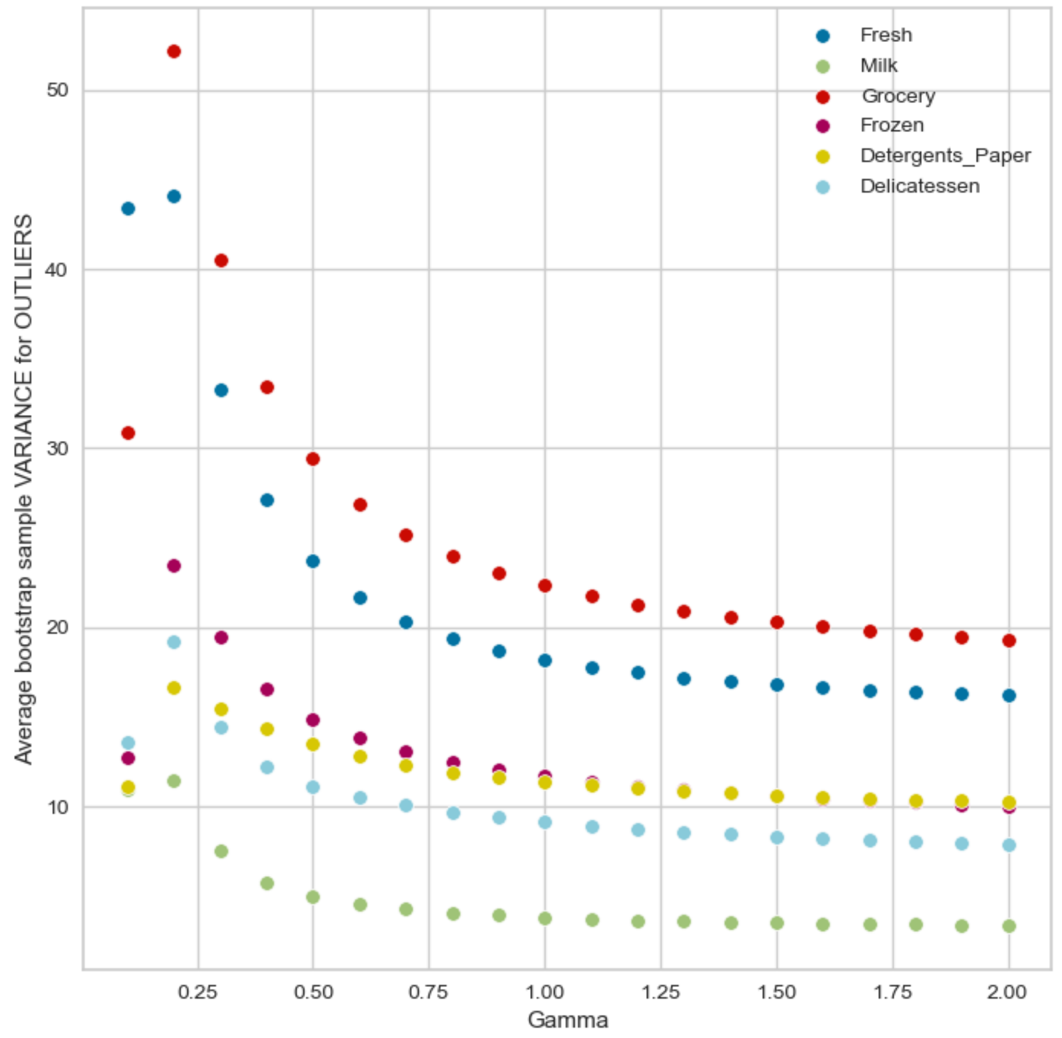
→ 440 x 1000 x 20 x 6 measurements

```
Fresh: all data: 0.95
       outliers: 0.7
Milk: all data: 0.96
       outliers: 1.0
Grocery: all data: 0.91
       outliers: 0.9
Frozen: all data: 0.98
       outliers: 0.9
Detergents_Paper: all data: 0.96
       outliers: 0.9
Delicatessen: all data: 0.98
       outliers: 0.9
```









4. Cluster Analysis

4.1. K parameter for K-means

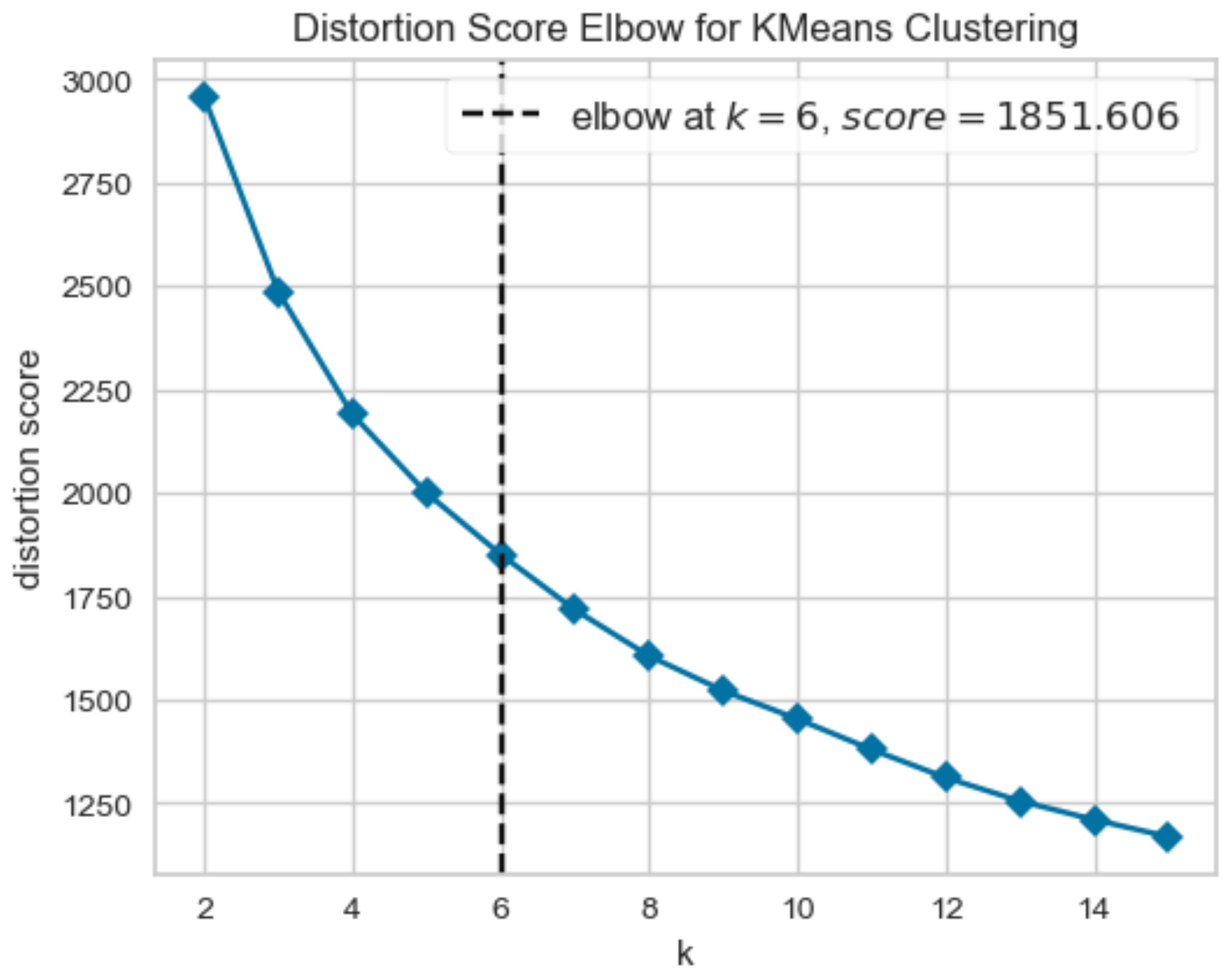
Intro

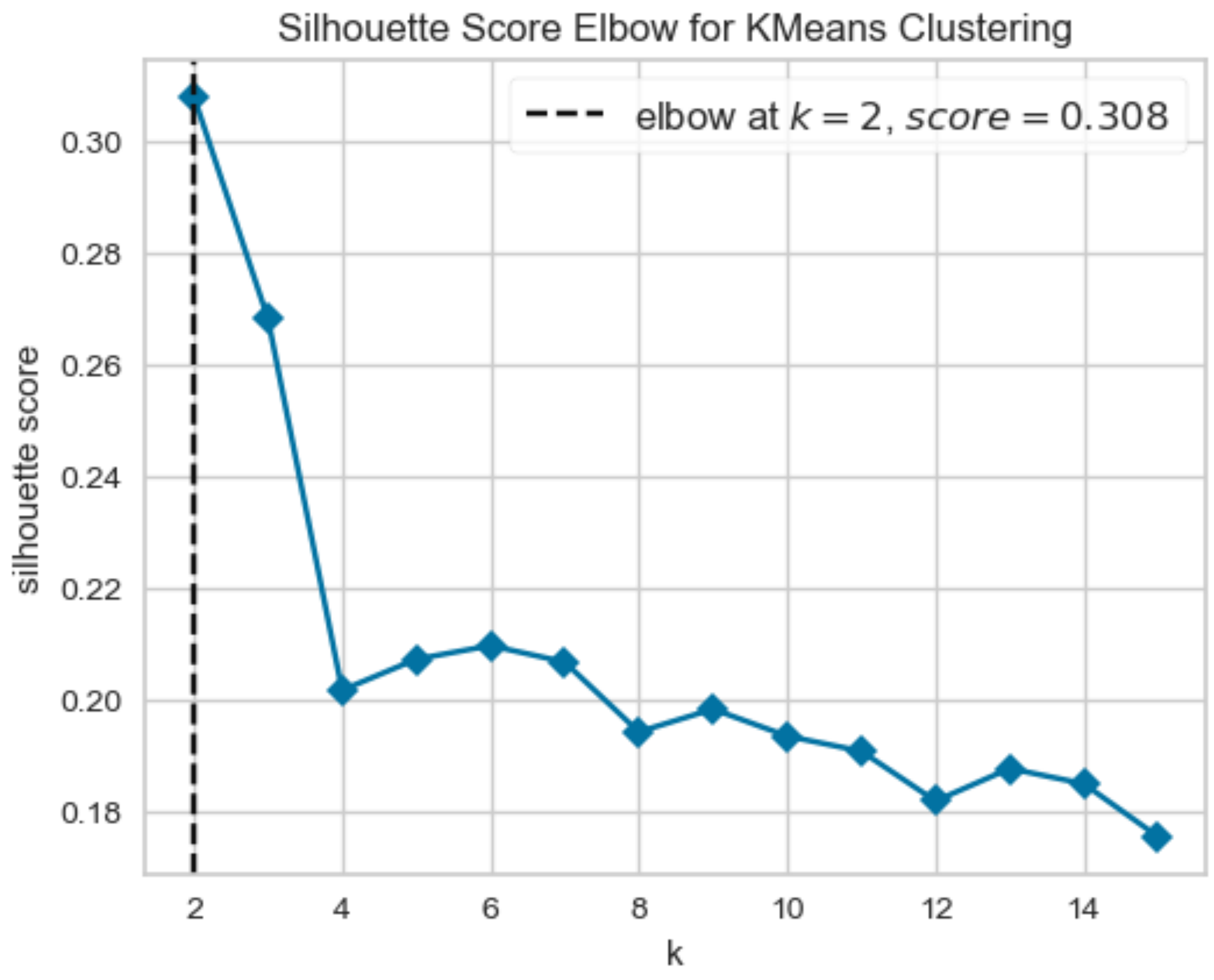
- The data does not appear to have natural cluster formations, DBSCAN algorithm was not fitting
- → Apply K-means clustering algorithm with greedy k-means++ algorithm over 100 initialisations
- Goal: partition customers into groups of relatively similar size that share tendencies in their purchases

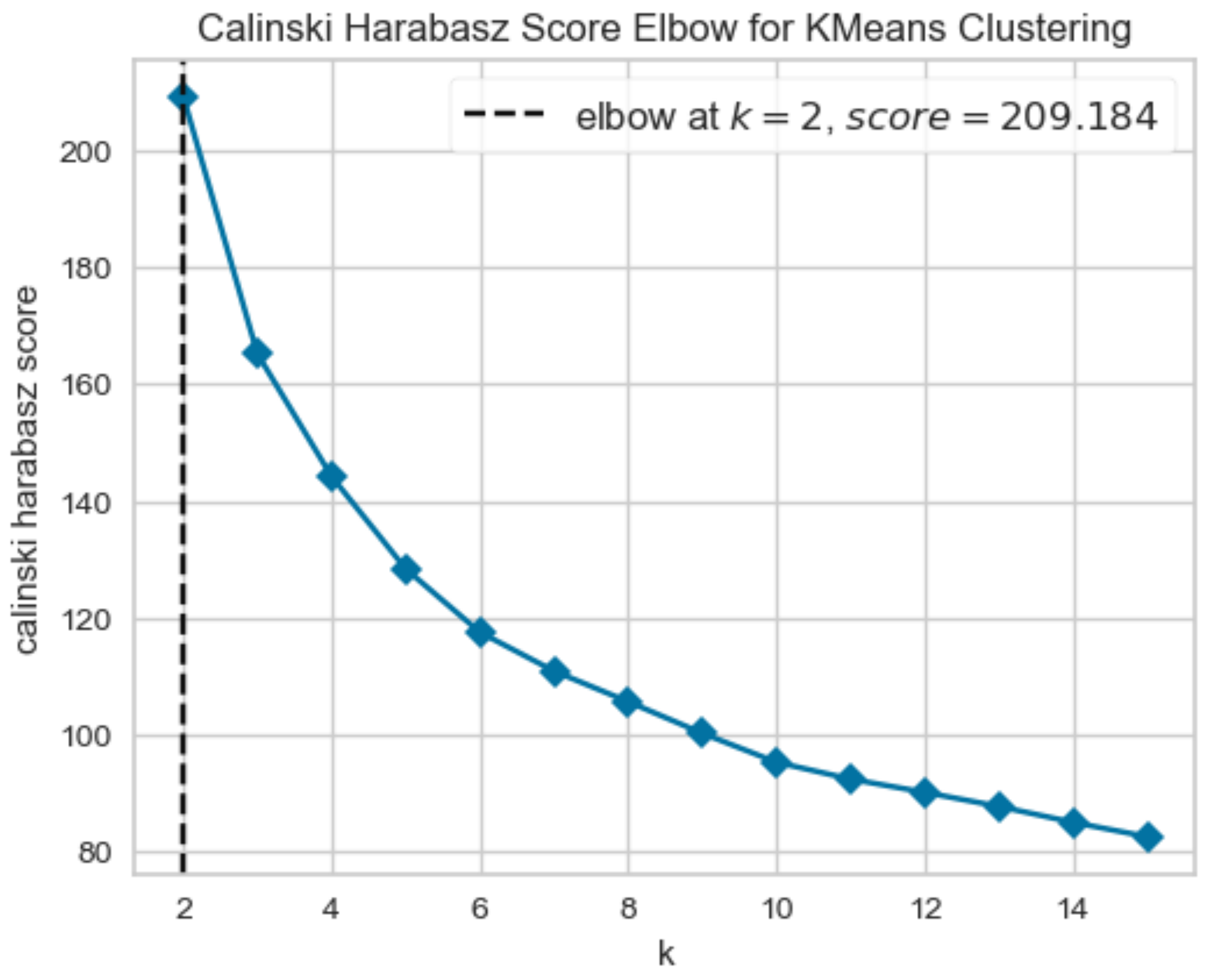
4.1. K parameter for K-means

Identify the Optimal Inflection Point for K in [2, 15]

- **Elbow (distortion score)**: the sum of squared distances from each point to its assigned center
- **Silhouette score**: the mean Silhouette Coefficient of all samples
- **Calinski-Harabasz score**: the ratio of dispersion between and within clusters

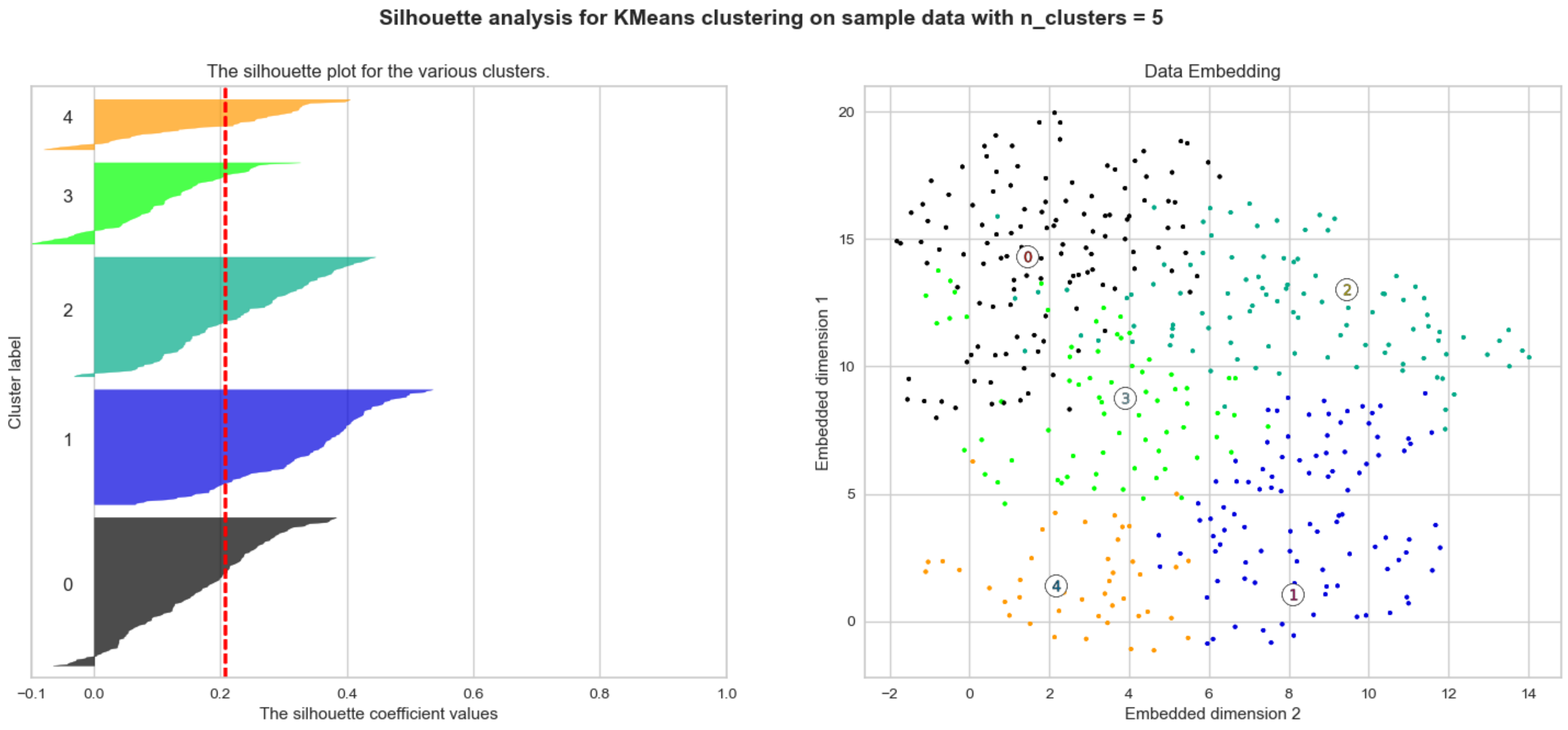




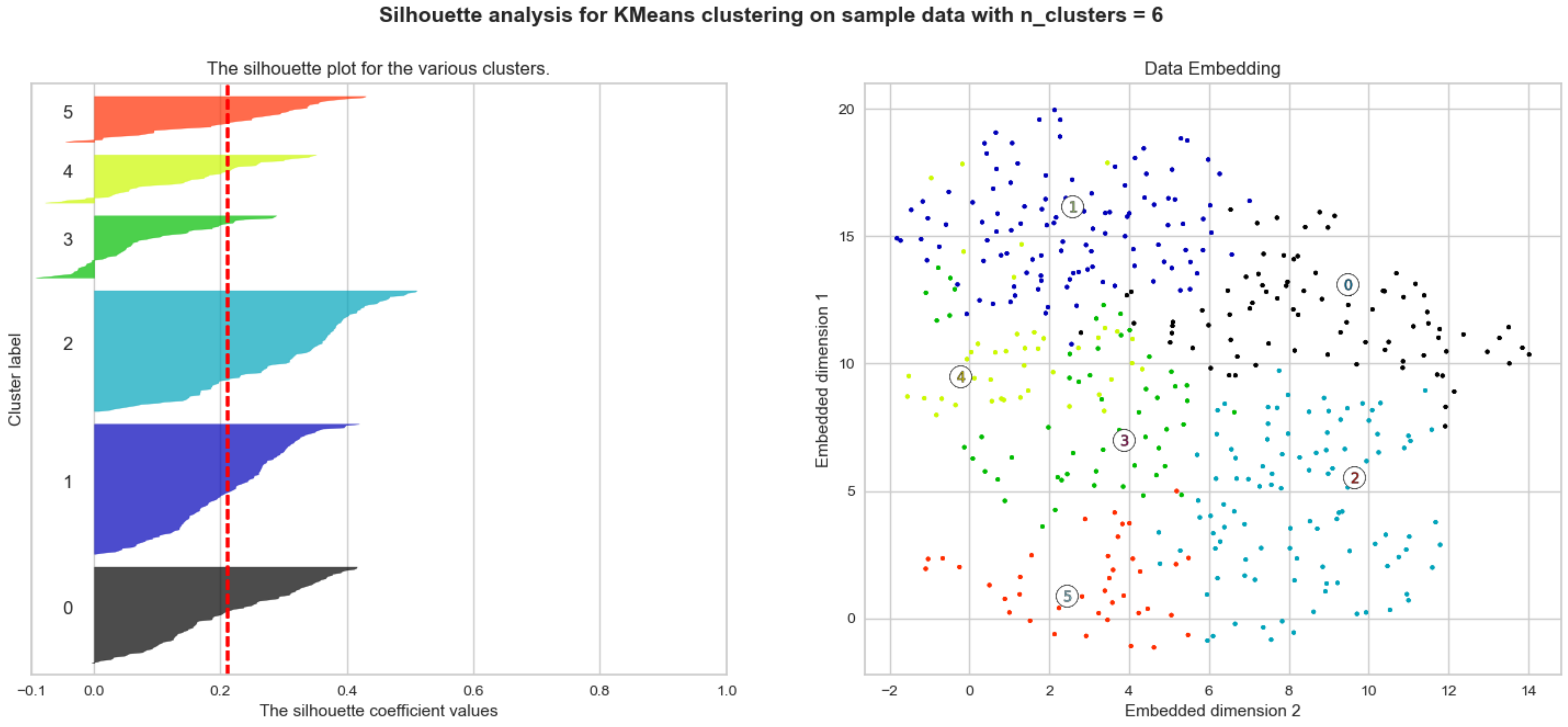


4.1. K parameter for K-means

Silhouette Plots for K in range [5, 6]

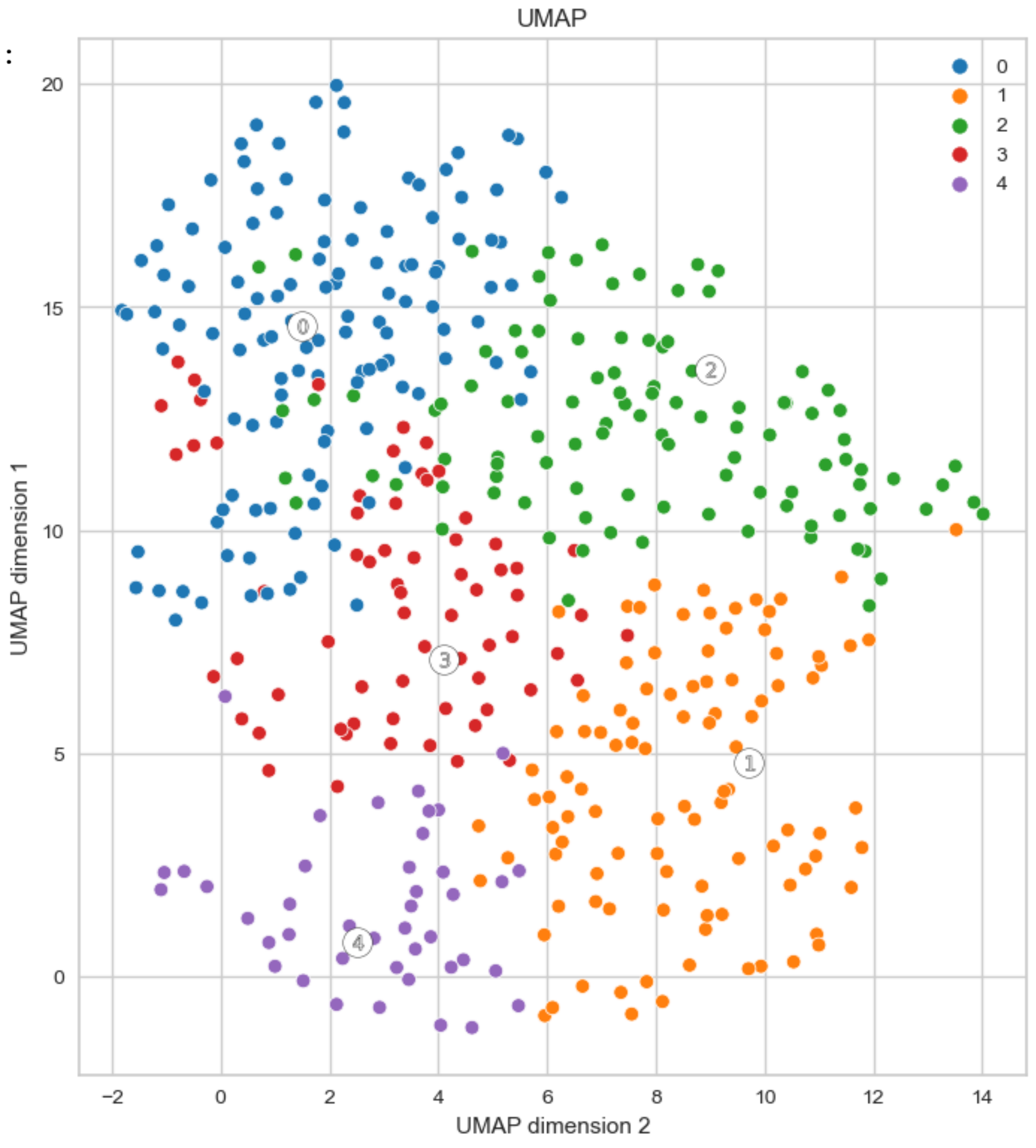


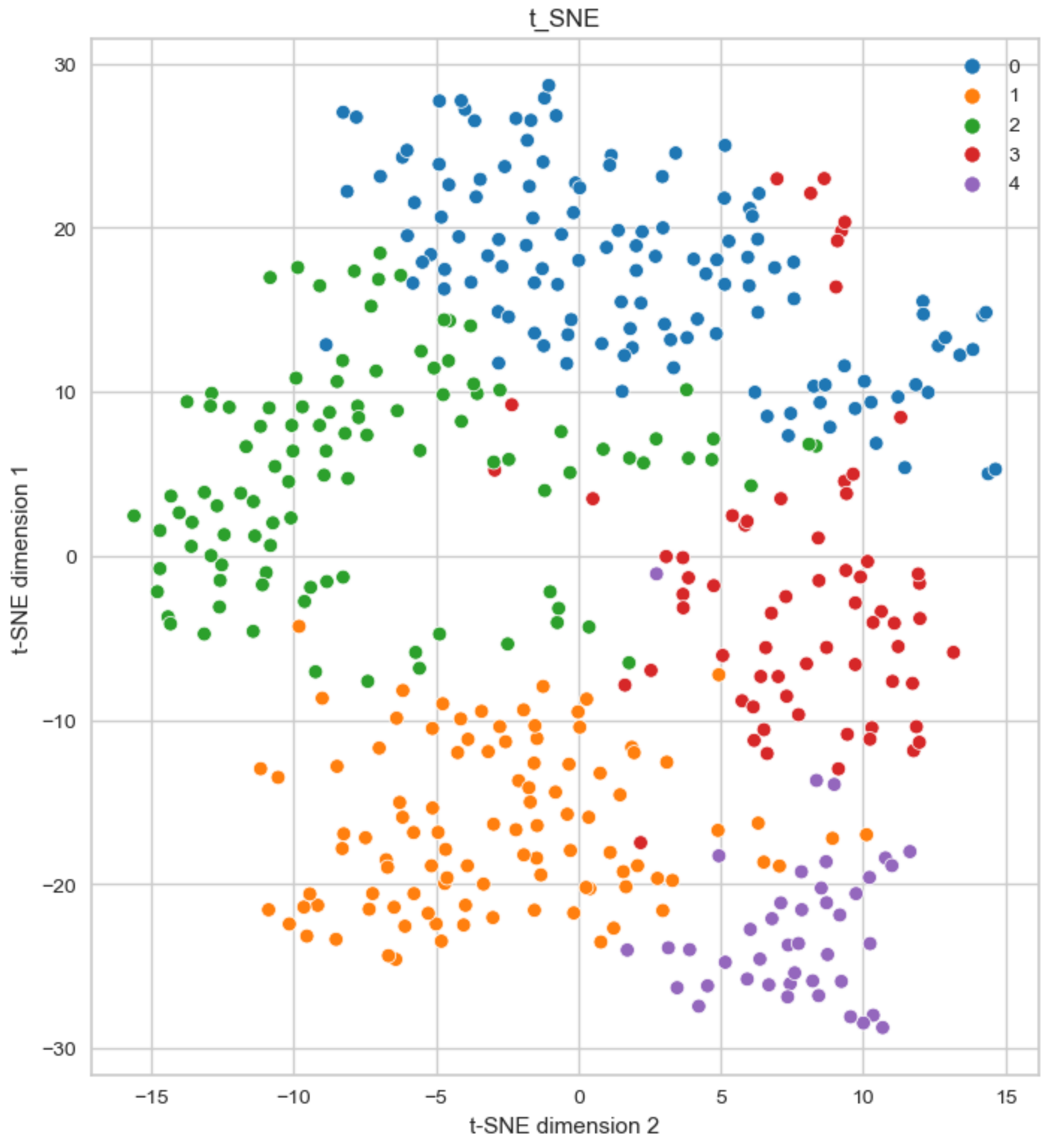

```
For n_clusters = 5 The average silhouette_score is : 0.20699
For n_clusters = 6 The average silhouette_score is : 0.21196
```



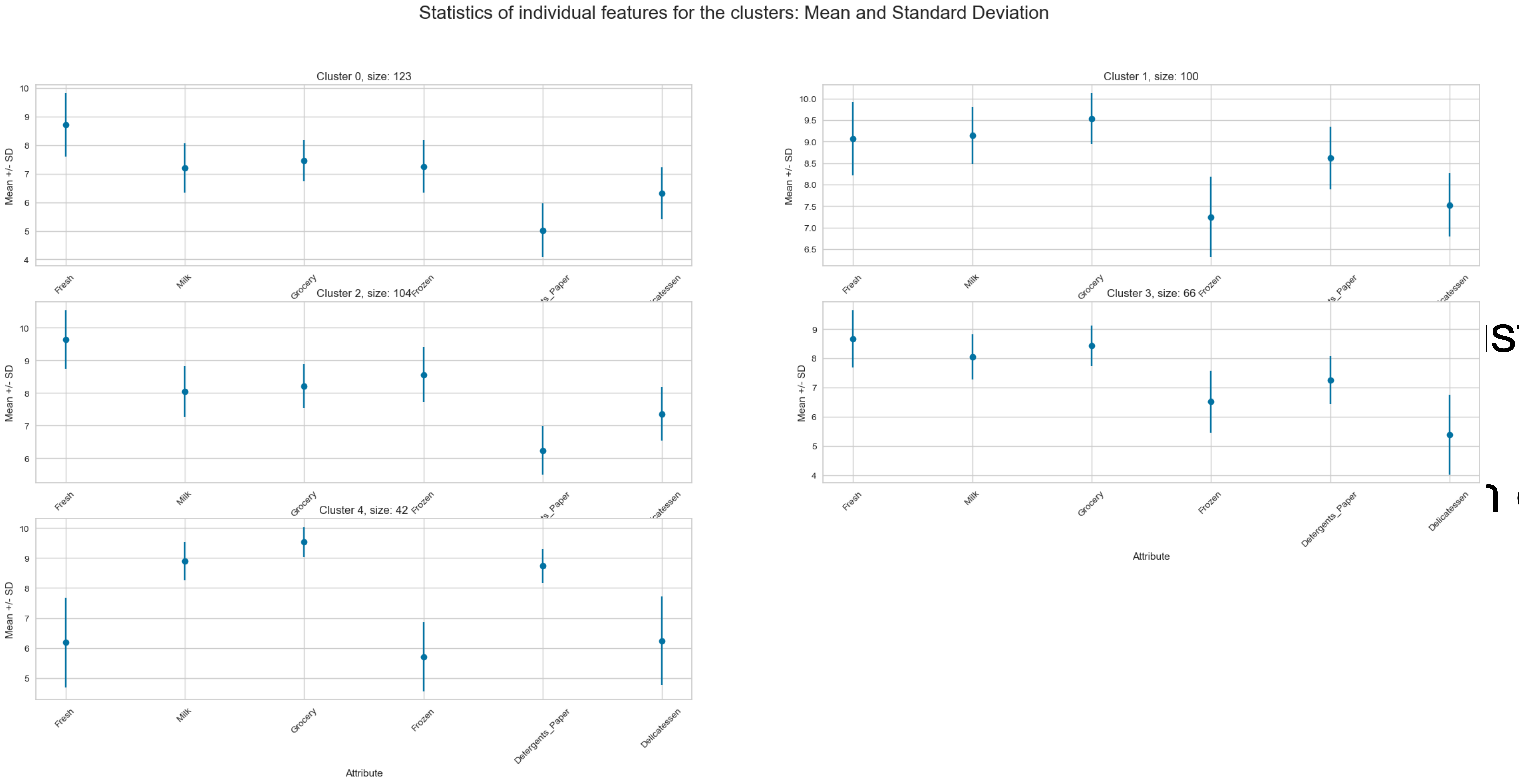
4.2. Clustering

```
k-Means cluster sizes:
Cluster: 0 : 123
Cluster: 1 : 100
Cluster: 2 : 104
Cluster: 3 : 66
Cluster: 4 : 42
```





4.3. Interpretation of the Clustering



- For ar … ster memb …
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4.3. Interpretation of the Clustering