Semi-Supervised Anomaly Detection Based on Quadratic Multiform Separation

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Abstract
In this paper we propose a novel method for semi-supervised anomaly detection (SSAD). Our classifier is named QMS22 as its inception was dated 2022 upon the framework of quadratic multiform separation (QMS), a recently introduced classification model. QMS22 tackles SSAD by solving a multi-class classification problem involving both the training set and the test set of the original problem. The classification problem intentionally includes classes with overlapping samples. One of the classes contains mixture of normal samples and outliers, and all other classes contain only normal samples. An outlier score is then calculated for every sample in the test set using the outcome of the classification problem. We also include performance evaluation of QMS22 against top performing classifiers using ninety-five benchmark imbalanced datasets from the KEEL repository. These classifiers are BRM (Bagging-Random Miner), OCKRA (One-Class K-means with Randomly-projected features Algorithm), ISOF (Isolation Forest), and ocSVM (One-Class Support Vector Machine). It is shown by using the area under the curve of the receiver operating characteristic curve as the performance measure, QMS22 significantly outperforms ISOF and ocSVM. Moreover, the Wilcoxon signed-rank tests reveal that there is no statistically significant difference when testing QMS22 against BRM nor QMS22 against OCKRA.

1. Introduction
Anomaly detection is the identification of rare items or outliers in a dataset. As a learning task, it may be supervised, semi-supervised, or unsupervised. Anomaly detection is an important data mining task that has been studied within diverse research areas. Inherently, outliers represent some kind of problem such as network intrusion, bank fraud, faulty equipment, or heart arrhythmia. Moreover, anomaly detection is often used in preprocessing to remove outliers from the dataset, which benefits the machine learning tasks that follow. There is a large number of survey papers on anomaly detection in the literature and we refer the readers to (Chandola et al., 2009; Taha and Hadi, 2019; Villa-Pérez et al., 2021) and the references therein.

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Burden in data preparation has been a barrier for companies to adopt AI. When it comes to anomaly detection, unsupervised algorithms require a minimal workload to prepare and audit the data. However, this is also associated with the price that a greater amount of data is needed and acceptable performance is harder to achieve.

In this paper, we consider semi-supervised anomaly detection (SSAD), where in addition to an unlabeled dataset, a set of normal samples is available for training. The problem is described as follows. Let $\mathcal{T}$ be a set consisting of only normal samples. Also let $\mathcal{S}$ denote an unlabeled dataset that contains both normal samples and outliers. It is assumed that $\mathcal{S}$ contains much more normal samples than outliers. Given a desired predicted positive (PP) $k$, the goal is to select $k$ samples from $\mathcal{S}$ in a way to grasp as many outliers as possible, i.e., to maximize the true positive rate (TPR) with respect to a fixed $k$. The choice for PP is application domain dependent. Contributing factors in determining its value include scrutiny cost for false positive samples and impact for neglecting false negative samples.

Our approach in solving SSAD is based upon quadratic multiform separation (QMS), a new concept recently proposed by Fan et al. (Fan et al., 2021). QMS is a mathematical model for classification in which one seeks pairwise separation of the so-called member sets using quadratic polynomials that satisfy certain cyclic conditions.

Evaluation of QMS will be hinged on the receiver operating characteristic curve, or ROC curve. The ROC curve is a very popular and powerful tool as a statistical performance measure in detection/classification theory and hypothesis testing. It is the graphical plot of true positive rate (TPR) against false positive rate (FPR). In addition to analyzing the strength and predictive power of a classifier, the ROC curve is also capable of determining optimal threshold settings as well as making model comparisons through the area under the curve (AUC).

The remainder of the paper is organized as follows: in Section 2 we give a brief introduction to the concept of QMS, in Section 3 we provide the design rationale behind which QMS was built upon, in Section 4 we lay out the details of QMS, in Section 5 we provide empirical results on the ninety-five datasets, in Section 6 we make comparisons with serveral top performing classifiers, and finally, the conclusion is given in Section 7.

2. Quadratic Multiform Separation

In this section, we give a brief introduction to the concept of quadratic multiform separation (QMS). We refer to (Fan et al., 2021) for more background on QMS.

The classification problem that QMS aims to solve is defined as follows. Let $\Omega \subset \mathbb{R}^p$ be a training set containing instances of $x$ from input-output pair $(x, y)$ generated by an unknown membership function $\mu : \Omega \rightarrow \mathcal{M}$. Here $x \in \mathbb{R}^p$ is a vector, $y$ is a class label selected from the set $\mathcal{M} = \{1, \ldots, m\}$ and $m$ is the number of possible classes. The problem is to find a classifier $\hat{\mu}(\cdot)$, serves as an approximation of $\mu(\cdot)$, by equating the behavior of $\hat{\mu}(\cdot)$ to the samples in the training set. For $i \in \mathcal{M}$, let $\Omega_i$ denote the member set defined by

$$\Omega_i = \{x \in \Omega : \mu(x) = i\}$$
A function in the form of \( f(x) = \|Ax-b\|^2 \) is called a member function, where \( q \) is a positive integer, \( A \in \mathbb{R}^{q \times p}, \ b \in \mathbb{R}^q \), and \( \| \cdot \| \) denotes the Euclidean norm. A function is a member function if and only if it is a (possibly degenerate) second order nonnegative polynomial.

QMS consists of \( m \) member functions \( f_1, \ldots, f_m \), which are constructed based on the training set \( \Omega \). Accordingly, a classifier \( \hat{\mu}(\cdot) \) defined by

\[
\hat{\mu}(x) \in \{ k : f_k(x) \leq f_i(x) \text{ for all } i \}
\]

can be realized. To facilitate the process of finding suitable member functions, a loss function that maps the member functions onto a real number must be defined. The QMS-specific loss function, denoted by \( \Phi \), is

\[
\Phi = \sum_{i \in \mathcal{M}} \phi_i
\]  

where, for \( i \in \mathcal{M} \), \( \phi_i \) denotes

\[
\phi_i = \sum_{x \in \Omega_i} \sum_{j \in \mathcal{M}, j \neq i} \max \left\{ \alpha, \frac{f_i(x)}{f_j(x)} \right\}
\]  

and \( \alpha \in [0, 1) \). Finally, the member functions are found via optimization by using the coordinate perturbation method (CPM). CPM adjusts the \( A_i \)’s and \( b_i \)’s (as they form the member functions \( f_i(x) = \|A_ix-b_i\|^2 \)) to reduce the loss function. The method works as follows. It successively minimizes along each and every entry of \( A_i \)'s and \( b_i \)'s, one at a time, to find a descending point. Along each entry, the method considers at most two nearby points, one along each of two opposite directions. It moves to a nearby descending point or otherwise does nothing if both nearby points do not produce a lower value for the loss function. The method then switches to the next entry and continues. With careful implementation, CPM can be extremely efficient and effective. In particular, there is no need to explicitly compute the loss function \( \Phi \) even once during the entire course of optimization. For each iteration, i.e., scanning all entries once for all \( A_i \)'s and \( b_i \)'s, the computation complexity of CPM is linear in \( p, q, m \), and the number of samples in \( \Omega \) (recall that \( p \) is the number of features and \( q \) is the row dimension of \( A_i \)).

In the sequel, a QMS task is referred to the task of finding \( m \) member functions with respect to \( m \) member sets by solving the underlying optimization problem.

3. Design Rationale

We consider the task of solving a trivial unsupervised anomaly detection problem (TUAD) in this section. The purpose here is to provide our decisions behind which QMS22 was built upon, and the reasons why those decisions were made. In this exercise, instead of tackling the problem with a simple-minded approach, we will solve it differently using ideas that can be crafted into a plausible scenario for SSAD.

Recall that \( \mathcal{S} \) is an unlabeled dataset containing both normal samples and outliers. Assume that the set \( \mathcal{T} \) is not present here. Let \( \mathcal{S}_0 \) and \( \mathcal{S}_1 \) respectively represent the set of normal samples and the set of outliers in \( \mathcal{S} \). The problem TUAD is to find the outliers
in $S$, given the assumption that $S_0$ is also available. It is clearly visible that the obvious solution is to check whether a sample lies in $S$ but not in $S_0$.

We would like to think TUAD in the context of QMS. Let us consider a QMS task with three classes and letting all members sets be equal to $S_0$, as shown in Figure 1. Also, we

\[\Omega_1 = S_0 \quad \Omega_2 = S_0 \quad \Omega_3 = S_0\]

Figure 1: First QMS task. All member sets are identical and do not contain outliers.

would like to inspect the expression of the corresponding loss function. To simplify the discussion, we choose $\alpha = 0$ in (2). It is then easily observed that the loss function, denoted by $\Phi_1$, is equal to

\[
\Phi_1 = \sum_{x \in S_0} \left\{ \left( \frac{f_1(x)}{f_2(x)} + \frac{f_2(x)}{f_1(x)} \right) + \left( \frac{f_1(x)}{f_3(x)} + \frac{f_3(x)}{f_1(x)} \right) \right. \\
\left. + \left( \frac{f_2(x)}{f_3(x)} + \frac{f_3(x)}{f_2(x)} \right) \right\}
\]

Each parentheses in (3) contains two terms that are reciprocal to each other. Therefore whenever possible, the optimization for keeping the loss function low will drive those terms in parentheses into equal values. That is to say, at the solution of minimizing $\Phi_1$, it is likely to observe that

\[f_1(x) = f_2(x) = f_3(x) \text{ for all } x \in S_0\] (4)

This result is perhaps expected due to the apparent symmetry of the problem.

Now we consider another QMS task as shown in Figure 2. It is identical to the first one except $\Omega_1$ is now equal to $S$. In this case, the loss function, denoted by $\Phi_2$, becomes

\[
\Phi_2 = \Phi_1 + \sum_{x \in S_1} \left\{ \frac{f_1(x)}{f_2(x)} + \frac{f_1(x)}{f_3(x)} \right\}
\]

The assumption that $S$ has much more normal samples than outliers comes to play an important role here. Consequently, at the solution of minimizing $\Phi_2$, it is likely to observe that

\[f_1(x) \approx f_2(x) \approx f_3(x) \text{ for } x \in S_0\]
• \( f_1(x) < f_2(x) \) and \( f_1(x) < f_3(x) \) for \( x \in S_1 \)

Therefore, the following function may serve as a good outlier score function:

\[
\eta(x) = \left( \frac{f_2(x) - f_1(x)}{f_1(x)} \right)^+ + \left( \frac{f_3(x) - f_1(x)}{f_1(x)} \right)^+ \tag{5}
\]

where given \( a \in \mathbb{R} \), \( a^+ = a \) if \( a > 0 \) and \( a^+ = 0 \) otherwise. In other words, the magnitude of \( \eta(x) \) provides an indication on how likely \( x \) is an outlier.

Now TUAD can be essentially solved as follows:

1. Carry out the second QMS task and obtain member functions \( f_1, f_2, \) and \( f_3 \).
2. For each \( x \in S \), compute its outlier score \( \eta(x) \).
3. Take first \( n_1 \) top outlier score samples as outliers, where \( n_1 \) is the cardinality of \( S_1 \).

4. Proposed Method

How is TUAD related to SSAD that we intend to solve? First, the set \( S_0 \) mentioned in TUAD is of course not available at our disposal. Nevertheless, the set \( T \) or a subset of \( T \) may serve as an approximation of \( S_0 \). Second, the sets \( \Omega_2 \) and \( \Omega_3 \) need not be identical. Instead, they can be individually an approximation of \( S_0 \).

For the QMS task to be involved in QMS22, the member sets \( \Omega_1, \ldots, \Omega_m \) will follow rules that \( |\Omega_1| \) is larger than \( |\Omega_2| \) and \( |\Omega_2| = \cdots = |\Omega_m| \), where \( |\cdot| \) denotes the cardinality. Under these circumstances, the corresponding classification problem naturally has imbalanced member sets to work with. In order to migrate the thought process given in Section 3 into realism, we will add a weight to \( \phi_1 \) to remedy this situation by changing the definition of loss function \( \Phi \) to

\[
\Phi = \frac{|\Omega_2|}{|\Omega_1|} \phi_1 + \sum_{i=2}^{m} \phi_i
\]

Finally, the outlier score for the general \( m \) is given by

\[
\eta(x) = \sum_{i=2}^{m} \left( \frac{f_i(x) - f_1(x)}{f_1(x)} \right)^+
\]

Figure 3: The QMS task solved in Algorithm 1.

We are now ready to present QMS22 as given in Algorithm 1. Under the framework of QMS, QMS22 amounts to solve a single \( m \)-class classification problem using both the
Algorithm 1 QMS22

Inputs:

- \( \mathcal{T} \): training set, consisting of only normal samples.
- \( \mathcal{S} \): test set, outliers within to be extracted.
- \( \mathcal{S}_0 \): subset of \( \mathcal{S} \), consisting of normal samples, used only in plotting the ROC curve.
- \( \mathcal{S}_1 \): subset of \( \mathcal{S} \), consisting of outliers, \( \mathcal{S} = \mathcal{S}_0 \cup \mathcal{S}_1 \), used only in plotting the ROC curve.
- \( m \): number of classes for the QMS task.

Outputs:

- ROC curve and its AUC.

1: (main step) Set \( \Omega_1 = \mathcal{S} \cup \mathcal{T} \). Shuffle \( \mathcal{T} \) well and divide it into \( m - 1 \) equal parts. Denote them as \( \mathcal{V}_2, \ldots, \mathcal{V}_m \), respectively. For \( i = 2, \ldots, m \), set \( \Omega_i = \mathcal{T} - \mathcal{V}_i \). Solve the QMS task with respect to \( \Omega_1, \ldots, \Omega_m \) as shown in Figure 3. Obtain the resulting member functions. Compute the outlier score for each of the samples in \( \mathcal{S} \) using the function \( \eta(\cdot) \) defined in (5).

2: (generate the ROC curve) For any \( \beta \geq 0 \), let \( \Lambda(\beta) \) be the subset of \( \mathcal{S} \) defined by

\[
\Lambda(\beta) = \{ x \in \mathcal{S} : \eta(x) \geq \beta \}
\]

Then the ROC curve is created by plotting

\[
\frac{|\Lambda(\beta) \cap \mathcal{S}_1|}{|\mathcal{S}_1|} \text{ versus } \frac{|\Lambda(\beta) \cap \mathcal{S}_0|}{|\mathcal{S}_0|}
\]

at various \( \beta \), from a sufficiently large value down to zero. The algorithm completes.

Finally, we address the computation complexity of QMS22. In view of the computation complexity of a generic QMS task mentioned in Section 2, it is not difficult to see that a similar conclusion can be made here. That is to say, the computation complexity of QMS22 depends linearly on \( n \) (the total number of samples in the training set and the test set), \( p \) (the number of features), \( m \) (a hyperparameter, the number of classes), \( q \) (a hyperparameter, the row dimension of \( A_i \)), and the iteration number in CPM. Typically, a
small $q$ (e.g., 5) and a small iteration number (e.g., 5) would suffice to produce a decent result.

5. Performance Evaluation: QMS22 Itself

In (Villa-Pérez et al., 2021), a thorough comparison was conducted to provide a broad empirical study with regard to ninety-five benchmark datasets from the KEEL repository\(^1\) (Alcalá-Fdez et al., 2011) and twenty-nine state-of-the-art SSAD classifiers. Those datasets are not related to a specific domain. Their experiments lead to the conclusion that, in terms of the AUC performance, the top four best players are BRM (Camiña et al., 2018), OCKRA (Rodríguez et al., 2016), ISOF (Sun et al., 2016; Liu et al., 2008), and ocSVM (Schölkopf et al., 1999). In this paper we will follow a similar experimental setup and compare QMS22 against those classifiers.

The performance evaluation runs on a computer with specification given in Table 1.

| Processor | Intel Core i7-8700K 3.70GHz × 12 |
| Memory   | 62.6 GB |
| OS Name  | Fedora 35 64-bit |

Table 1: Specification of the computer where performance evaluation is performed.

The code is implemented in the C language using double precision arithmetic. It only invokes a single user thread and does not use any GPU. The source code will be available publicly in a later time.

The ninety-five datasets are illustrated in Table 6. Each dataset contains five related datasets (namely, 5-fold datasets) to perform cross validation. Each of the 5-fold datasets consists of a training set and a test set. Their size ratio is about 4:1. In our SSAD setup, all outliers in the training set must be removed prior to the classifier. Therefore we obtain total of 5 AUC’s for the 5-fold datasets. The representative AUC for the dataset is then the average of those 5 AUC’s.

Before sending the data to QMS22, every dataset is preprocessed as follows:

- Categorical data is converted to a numeric form using OneHotEncoder\(^2\).
- Each feature variable is normalized so that its maximal absolute value among all samples in the training set is 255.

The hyperparameters used in QMS22 are listed in Table 2. Finally, The AUC and CPU time results are summarized in Table 6.

6. Performance Evaluation: Comparison

In this section we compare QMS22 against four above-mentioned classifiers. The numerical result pertaining to those classifiers is either taken directly from (Villa-Pérez et al., 2021) or

\(^1\) http://sci2s.ugr.es/keel/datasets.php.
\(^2\) https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.OneHotEncoder.html.
| Description                                | Value                                |
|-------------------------------------------|--------------------------------------|
| number of classes ($m$)                   | 7                                    |
| row dimension of $A_i$ ($q$)              | 10                                   |
| threshold in loss function ($\alpha$)     | 0.5                                  |
| CPM: number of iterations executed        | 60                                   |
| CPM: distance to nearby entry in $A_i$    | 1                                    |
| CPM: distance to nearby entry in $b_i$    | 255                                  |
| CPM: initial condition of $A_i$           | zero matrix                          |
| CPM: initial condition of $b_i$           | 25500 at first entry and zero elsewhere |

Table 2: Hyperparameters selected in QMS22 (within the QMS task).

borrowed from the authors of (Villa-Pérez et al., 2021), courtesy of M.E. Villa-Pérez. To put the comparison in perspective, we will focus on boxplot (Mcgill et al., 1978), average AUC, Wilcoxon signed-rank test (Woolson, 2008; Pagano and Gauvreau, 2018), and computation complexity.

### 6.1 Boxplots

![Boxplot Image](image)

Figure 4: Boxplots using all datasets.

A boxplot is a method for graphically demonstrating the locality, spread and skewness groups of numerical data through their quartiles. It displays the distribution of the data
Based on a summary of five values: minimum, first quartile, median, third quartile, and maximum.

Based on the plots given in Figure 4, we see that:

- BRM slightly outperforms QMS22.
- QMS22 slightly outperforms OCKRA.
- QMS22 outperforms ISOF and ocSVM.

6.2 Average AUC and standard deviation

| Classifier | Average AUC | STD |
|------------|-------------|-----|
| QMS22      | 0.8252      | 0.1483 |
| BRM        | 0.8347      | 0.1442 |
| OCKRA      | 0.8110      | 0.1491 |
| ISOF       | 0.7785      | 0.1410 |
| ocSVM      | 0.7616      | 0.1493 |

Table 3: Average AUC and the standard deviation (STD) using all datasets.

Based on the average AUC given in Table 3, it leads to the same observations as before.

6.3 Wilcoxon signed-rank tests

| Comparison       | $R^+$ | $R^-$ | Null-hypothesis | p-value |
|------------------|-------|-------|-----------------|---------|
| QMS22 vs. BRM    | 2086  | 2379  | Not rejected    | > 0.5   |
| QMS22 vs. OCKRA  | 2446  | 2019  | Not rejected    | > 0.4   |
| QMS22 vs. ISOF   | 3470  | 1090  | Rejected        | < 0.00001 |
| QMS22 vs. ocSVM  | 3481  | 984   | Rejected        | < 0.00001 |

Table 4: Wilcoxon signed-ranks tests using all datasets.

The Wilcoxon signed-rank tests are conducted to verify the null-hypothesis that the performances of each paired classifiers, on all datasets, are similar statistically. Table 4 shows the comparisons of QMS22 against BRM, OCKRA, ISOF, and ocSVM, respectively. Here $R^+$ is the sum of ranks for the datasets on which QMS22 outperforms the paired classifier, and $R^-$ the sum of ranks for the opposite. With the chosen significance level 0.05, the result of each test and p-value are stated.

Based on the test results given in Table 4 and everything above, we conclude that:

- There is no statistically significant difference between QMS22 and BRM, and between QMS22 and OCKRA.
- QMS22 significantly outperforms ISOF and ocSVM.
6.4 Computation complexities

The computation complexities for various classifiers are summarized in Table 5.

| Classifier | Complexity                |
|------------|---------------------------|
| QMS22      | $O(n)$                    |
| BRM        | $O(n^2)$                  |
| OCKRA      | Not reported              |
| ISOF       | $O(n)$                    |
| ocSVM      | Convex quadratic programming |

Table 5: Computation complexities reported by authors in their work.

7. Conclusion

In this paper we propose a simple, of low computation complexity, and yet effective classifier QMS22 for semi-supervised anomaly detection. We empirically evaluate its performance on ninety-five imbalanced benchmark datasets taken from the KEEL repository and compare against the classifiers BRM, OCKRA, ISOF, and ocSVM, which are the top four performing classifiers on the same collection of datasets. Our study shows that QMS22 significantly outperforms ISOF and ocSVM. Furthermore, according to the Wilcoxon signed-rank tests, QMS22 exhibits no statistically significant difference to BRM and OCKRA, respectively.

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Table 6: Datasets. $n$, $p$, AUC, and $t$ respectively stand for number of samples, number of features, AUC, and cpu time in second.

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