

Outlier Preservation by Dimensionality Reduction Techniques

Martijn Onderwater^{1,2,*}

¹ Center for Mathematics and Computer Science (CWI)
Science Park 123, 1098 XG, Amsterdam,
The Netherlands.

E-mail: m.onderwater@cwi.nl

Fax: +31 (0)20 592 4199

² VU University, Faculty of Sciences
Amsterdam, The Netherlands.

*Corresponding author

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Abstract

Sensors are increasingly part of our daily lives: motion detection, lighting control, and energy consumption all rely on sensors. Combining this information into, for instance, simple and comprehensive graphs can be quite challenging. *Dimensionality reduction* is often used to address this problem, by decreasing the number of variables in the data and looking for shorter representations. However, dimensionality reduction is often aimed at normal daily data, and applying it to events deviating from this daily data (so-called *outliers*) can affect such events negatively. In particular, outliers might go unnoticed. In this paper we show that dimensionality reduction can indeed have a large impact on outliers. To that end we apply three dimensionality reduction techniques to three real-world data sets, and inspect how well they preserve outliers. We use several performance measures to show how well these techniques are capable of preserving outliers, and we discuss the results.

Keywords: dimensionality reduction; outlier detection; multidimensional scaling; principal component analysis; t-stochastic neighbourhood embedding; peeling; F1-score; Matthews Correlation; Relative Information Score; sensor network.

Biographical notes: Martijn Onderwater is a Ph.D. student at the Center for Mathematics and Computer Science (Amsterdam, The Netherlands), and at VU University (Amsterdam, The Netherlands). He received a M.Sc. degree in Mathematics (2003) from the University of Leiden (The Netherlands), and a M.Sc. degree in Business Mathematics & Informatics (2010, Cum Laude) from VU University Amsterdam. He also has several years of commercial experience as a software engineer. His research focuses on sensor networks, and his interests include dimensionality reduction, outlier detection, caching in sensor networks, Markov decision processes, correlations in sensor data, and middleware for sensor networks.

1 Introduction

Recent technological developments have resulted in a broad range of cheap and powerful sensors, enabling companies to use sensor networks in a cost-effective way. Consequently, sensor networks will increasingly become part of our daily life. One can for instance envision a house with sensors related to smoke detection, lighting control, motion detection, environmental information, security issues, and structural monitoring.

Combining all this information to actionable insights is a challenging problem. For instance, in the event of a burglary in a house, the sensors involved in motion detection, environmental monitoring, and security all yield useful information. Providing a short insightful summary that helps users identify the event and take appropriate action is essential. *Dimensionality reduction* (DR) is a family of techniques aimed at reducing the number of variables (dimensions) in the data and thus making the data set smaller. In essence, it helps identify what is important, and what is not.

However, in practise dimensionality reduction often yields some loss of information, and applications might be affected by this loss. For instance, the burglary mentioned before is a (hopefully) rare event that is different from normal patterns in the sensor data (i.e. a so-called *outlier*). Unfortunately, DR-methods often lose outliers among the regular sensor data. Figure 1 illustrates this situation using a two-dimensional data set with an outlier near the top-left corner. When dimensionality is reduced by projecting all points onto a line, the outlier is mapped into the center of the reduced data set (the middle arrow in Figure 1), and is thus no longer an outlier. So dimensionality reduction might lose outliers among regular points, causing problems for applications relying on the

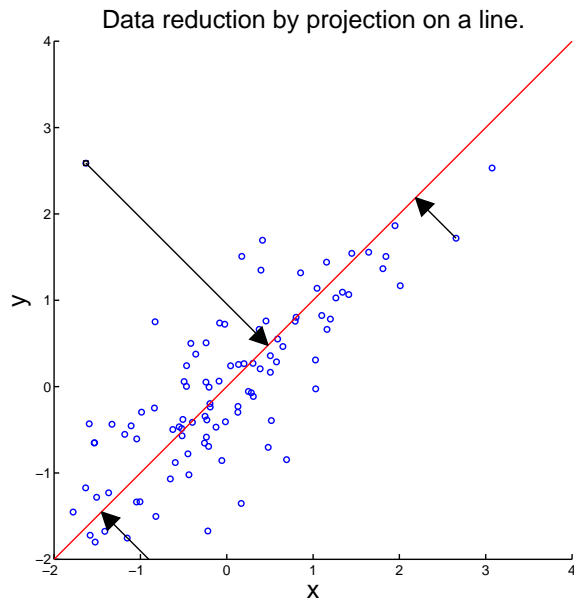


Figure 1. A two-dimensional data set reduced to one dimension, with an outlier (middle arrow) mapped to the center of the reduced data set

detection of outliers. The example in Figure 1 illustrates one DR-technique, but many others exist, each affecting outliers differently.

In this paper we show that DR-techniques affect outliers, by measuring their capability to preserve outliers. For this purpose we describe three well-known DR-techniques that are relevant for a broad audience, and apply them to several real-world data sets from a sensor-related context. For each DR-technique we capture its capability to preserve outliers in three performance measures, and compare the results. From the three techniques we will identify the one with the best performance, and discuss the intuitions behind the scores.

Research on both dimensionality reduction and outlier detection is abundant. An overview of dimensionality reduction techniques can be obtained from [Carreira-Perpinán \(1997\)](#); [Fodor \(2002\)](#); [Gupta and Kapoor \(2012\)](#); [Kline and Galbraith \(2009\)](#); [Onderwater \(2010\)](#); [Van der Maaten et al. \(2009\)](#). For outlier detection, we refer readers to, e.g., [Agyemang et al. \(2006\)](#); [Hodge and Austin \(2004\)](#); [Maalouf and Trafalis \(2011\)](#); [Zhang et al. \(2010, 2007\)](#). Certain specific topics such as intrusion detection [Gogoi et al. \(2011\)](#) and fraud detection [Becker et al. \(2010\)](#); [Phua et al. \(2005\)](#) are closely related to outlier detection. In [Muñoz and Muruzábal \(1998\)](#) the authors consider Kohonen’s Self Organizing Maps (SOM, [Kohonen \(2001\)](#)) and how this DR-technique can be used to identify outliers. [Harmeling et al. \(2006\)](#) illustrate the effect of outlier-removal on Isomap ([Tenen-](#)

baum et al. (2000)), another DR-technique. Chakrabarti and Mehrotra (2000) look at local DR, where reduction is applied to previously identified clusters. Outlier detection occurs as part of the cluster-identification phase. Non of these papers, however, look at outlier *preservation* by DR-techniques, as discussed in this paper. In Escalante (2005), the authors compare multiple outlier detection methods on various data sets, including one data set with its dimensionality reduced. As in our paper, their analysis also suggests that outlier detection is affected by dimensionality reduction, although they only use one DR-methods and one performance measure. The paper by Nguyen et al. (2010) has a setup that is close to our approach: four DR-methods (*feature extraction* methods in their terminology) are applied to three data sets, and the performance (using one score measure) is inspected for two outlier detection methods. However, their DR-methods are selected from the Feature Extraction domain, and are not well-known in the DR-community.

The structure of the paper is as follows: Section 2 describes the DR-techniques, Section 3 contains the outlier detection method as well as the performance measures. Then, in Section 4 we describe the data sets that we use in the experiments. Section 5 shows the output of the experiments and discusses the results, followed by conclusions, recommendations, and ideas for further research in Section 6.

2 Dimensionality reduction techniques

Denote by n the number of measurements and by d the number of sensors producing the measurements. The number of sensors is known as the *dimension* of the data, and DR-techniques aim to lower this dimension to a smaller value. More formally, if the measurements are vectors $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$, then DR-techniques try to find points $\mathbf{y}_1, \dots, \mathbf{y}_n \in \mathbb{R}^{d'}$ with $d' < d$. Dimensionality reduction is often used for, e.g., visualisation Li (1992); Tsai (2012), as a preprocessing step for further analysis UmaMaheswari and Rajaram (2009); Garg and Murty (2009); Ravi and Pramodh (2010), or for computational efficiency Hahn et al. (2003); Dai et al. (2006).

This section describes three well-known and often used DR-techniques: *Principal Component Analysis* (PCA), *Multidimensional Scaling* (MDS), and *t-Stochastic Neighbourhood Embedding* (t-SNE).

2.1 Principal Component Analysis

Principal Component Analysis was initially proposed by [Pearson \(1901\)](#). It finds a low dimensional representation of the data with minimal loss of variation in the reduced data set. The first step in PCA is a linear change of base from $\mathbf{x}_1, \dots, \mathbf{x}_d \in \mathbb{R}^d$ to $\mathbf{u}_1, \dots, \mathbf{u}_d \in \mathbb{R}^d$, where \mathbf{u}_1 is aligned with the direction of maximum variance in the data. Vectors \mathbf{u}_i ($2 \leq i \leq d$) are also lined up with the direction of maximum variance, but constrained to be perpendicular to $\mathbf{u}_{i-1}, \dots, \mathbf{u}_1$. The \mathbf{u}_i vectors are called *Principal Components*.

Suppose that the n data points are in the $n \times d$ matrix X , then the vectors \mathbf{u}_i are found by calculating the eigenvectors of the correlation matrix (C) ([Johnson and Wichern \(2002\)](#)). The eigenvalues of C correspond to the amount of variance explained by the corresponding eigenvectors. Dimensionality reduction is achieved by omitting eigenvectors $\mathbf{u}_{d'+1}, \dots, \mathbf{u}_d$ once eigenvalues $\lambda_1, \dots, \lambda_{d'}$ explain enough of the variance of the data set. Summarized, the process works as follows:

- Construct the data matrix X .
- Compute the correlation matrix C .
- Find the eigenvalues and eigenvectors of C .
- Determine d' such that $\lambda_1, \dots, \lambda_{d'}$ explain enough of the variance of the data.
- Construct matrix $\hat{U} = [\mathbf{u}_1 \dots \mathbf{u}_{d'}]$.
- Reduce dimension by computing $\hat{X} = X\hat{U}^T$.

More details on PCA can be found in, e.g., [Härdle and Simar \(2012\)](#); [Johnson and Wichern \(2002\)](#); [Lattin et al. \(2003\)](#); [Tabachnick and Fidell \(2001\)](#); [Yoon \(2003\)](#).

2.2 Multidimensional Scaling

Multidimensional Scaling is the name for a family of dimensionality reduction techniques based on preserving distances in the data set. The *classical* version of Multidimensional Scaling finds points $\mathbf{y}_1, \dots, \mathbf{y}_n \in \mathbb{R}^{d'}$ in a low dimensional space that minimize

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \sum_{i=1}^n \sum_{j=1}^n (\|\mathbf{x}_i - \mathbf{x}_j\| - \|\mathbf{y}_i - \mathbf{y}_j\|)^2. \quad (1)$$

Here $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ are the high dimensional points, and $\|\cdot\|$ is the Euclidean distance in the respective space. The classical version of MDS is equivalent to PCA, see for instance Ghodsi (2006). Other members of the MDS family use a different distance measure or a different quantity to optimize than Eq. (1). We use a version of MDS with the so-called *squared stress* criterion

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \frac{\sum_{i=1}^n \sum_{j=1}^n (\|\mathbf{x}_i - \mathbf{x}_j\|^2 - \|\mathbf{y}_i - \mathbf{y}_j\|^2)^2}{\sum_{i=1}^n \sum_{j=1}^n \|\mathbf{x}_i - \mathbf{x}_j\|^4}. \quad (2)$$

For the distance measure $\|\mathbf{x}_i - \mathbf{x}_j\|$ we do not use the Euclidean distance measure as in the classical version of MDS. To see why, note that MDS with the Euclidean distance is sensitive to natural variations in the data. Consider, for instance, a data set consisting of two columns, one with values uniformly drawn from $[1000 - 2000)$ and one with values drawn from $[0, 1)$. Clearly, all values in the first column are several orders of magnitude larger than those in the second column. When minimizing the quantity in Eq. (1) the procedure focuses on the elements of the first column, since that brings it closest the minimum. In essence, the second column is ignored and MDS is biased towards the first column.

To overcome this problem the Euclidean distance is replaced by the *Mahalanobis* distance (Mahalanobis (1936))

$$\|x_i - x_j\|_M = \sqrt{(\mathbf{x}_i - \mathbf{x}_j) \Sigma^{-1} (\mathbf{x}_i - \mathbf{x}_j)^T}, \quad (3)$$

where Σ is the covariance matrix. By including the covariance matrix in the distance measure, the natural variations in the data are removed and thus MDS is unbiased with respect to dimensions. Eq. (1) then becomes

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \frac{\sum_{i=1}^n \sum_{j=1}^n (\|\mathbf{x}_i - \mathbf{x}_j\|_M^2 - \|\mathbf{y}_i - \mathbf{y}_j\|^2)^2}{\sum_{i=1}^n \sum_{j=1}^n \|\mathbf{x}_i - \mathbf{x}_j\|_M^4}. \quad (4)$$

Note that the Mahalanobis distance is only used for the high-dimension points \mathbf{x}_i , because the low-dimensional points \mathbf{y}_i are found by the minimization.

2.3 t-Stochastic Neighbourhood Embedding

2.3.1 Stochastic Neighbourhood Embedding

t-Stochastic Neighbourhood Embedding is a variation on *Stochastic Neighbourhood Embedding* (SNE), first proposed by [Hinton and Roweis \(2002\)](#). SNE presents the novel idea of defining a probability that two points are neighbours. Mapping to low dimensional space is achieved by choosing points that preserve these probabilities. They define Gaussian-inspired probabilities $p_{i|j}$ in high dimensional space, representing the probability of point \mathbf{x}_i being a neighbour of a given point \mathbf{x}_j , as

$$p_{i|j} = \frac{e^{-\|\mathbf{x}_i - \mathbf{x}_j\|_M^2 / 2\sigma_i^2}}{\sum_{k \neq i} e^{-\|\mathbf{x}_i - \mathbf{x}_k\|_M^2 / 2\sigma_i^2}}. \quad (5)$$

The parameter σ_i is set by hand or determined with a special search algorithm. Note how we again employ the Mahalanobis distance for the high-dimensional points. In low dimensional space, probabilities similar to those in Eq. (5) are defined as

$$q_{i|j} = \frac{e^{-\|\mathbf{y}_i - \mathbf{y}_j\|^2}}{\sum_{k \neq i} e^{-\|\mathbf{y}_i - \mathbf{y}_k\|^2}}. \quad (6)$$

The parameter σ_i is not necessary here, because it would only lead to a rescaling of the resulting low dimensional points \mathbf{y}_i . The \mathbf{y}_i are then found by minimizing the Kullback-Leibler divergence of these two probability distributions

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \sum_i \sum_j p_{i|j} \log \frac{p_{i|j}}{q_{i|j}}. \quad (7)$$

Minimization of Eq. (7) can be done with, e.g., the gradient descent algorithm, or the scaled conjugate gradients procedure.

2.3.2 t-SNE

In [Van der Maaten and Hinton \(2008\)](#) the authors propose t-SNE, which differs from SNE in two aspects. First, note that the probabilities in Eq. (5) are not necessarily symmetric, i.e., $p_{i|j}$ and $p_{j|i}$ do not need to be equal. This

complicates minimization of Eq. (7), because it has twice as many variables as in the symmetric case. In t-SNE, these probabilities are redefined to be symmetric:

$$p_{ij} = \frac{p_{i|j} + p_{j|i}}{2n}.$$

Additionally, this ensures that $\sum_j j p_{ij} > 1/2n$ so that each point (including outliers) have a significant contribution to the cost function. The second change proposed for t-SNE concerns the q_{ij} . Instead of using Gaussian-style probabilities as in Eq. (6), t-SNE uses probabilities inspired by the Student t-distribution (with one degree of freedom):

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq i} (1 + \|\mathbf{y}_i - \mathbf{y}_k\|^2)^{-1}}.$$

This distribution has heavier tails than the Gaussian used by SNE, so should map nearby high dimensional points less nearby in low dimensional space than SNE. A justification for this approach comes from the so-called *Crowding problem*: there is much more room in high dimensional space for points, so in a low dimensional representation data points tend to be 'squeezed' together. By using the Student t-distribution, these crowded points are placed just a bit further apart. Low dimensional points are still found by optimizing the Kullback-Leibler divergence

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_n} \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}. \quad (8)$$

3 Experimental setup

We adopt the following experimental setup when investigating dimensionality reduction for outlier preservation:

1. Modify each data set so that it has zero mean and unit variance. This is a common preprocessing step for experimental data.
2. Find outliers in the high-dimensional (centered and scaled) data set.
3. Reduce the data set to two dimensions.
4. Again look for outliers, this time in the low-dimensional data.

5. Compute a score showing how each DR-methods performs on the data set.

We apply this setup to the DR-techniques from Section 2 and to a number of real-world data sets, described later in Sections 4.1-4.3. The sections below describe the technique that we use for outlier detection, and three performance measures that we use to assess how well outliers are preserved. For the DR-techniques we used Matlab implementations available in the *Dimensionality Reduction Toolbox* by Van der Maaten (2009).

3.1 Onion Peeling

The idea of *Onion Peeling*, or Peeling in short, is to construct a convex hull around all the points in the data set and then find the points that are on the convex hull. These points form the first ‘peel’ and are removed from the data set. Repeating the process gives more peels, each containing a number of points.

This technique can be modified for finding outliers. The largest outlier in the data set is on the first peel, so by inspecting the total distance of each point on the hull to all other points in the data set, we can find the one with the largest total distance. Removing this point from the data set and repeating the process gives new outliers. The decrease in volume of the convex hull after removing an outlier is used as a stop criterion. Once the volume decreases by a fraction less than α ($0 \leq \alpha \leq 1$), we stop looking for outliers. Although with this criterion there is no guarantee that all outliers are found, it does assure that all found points are outliers. In our experiments we set $\alpha = 0.005$. Peeling is outlined in algorithm 1.

Algorithm 1: Peeling
<ol style="list-style-type: none">1. Calculate the convex hull around all the points in the data set.2. Find the point on the hull with the largest (Mahalanobis) distance to all other points in the data set.3. Remember the outlier and remove it from the data set.4. Calculate the new convex hull, and check if the stop criterion is reached. If so, stop, otherwise continue with step 2.

3.2 Measuring performance

After running the experiment for one data set and one DR-method, we need to quantify the performance of this method with respect to the preservation of outliers. In order to do so, we assign each point to one of four groups:

- True Positive (TP). The point is an outlier both before and after DR.
- False Positive (FP). The point is not an outlier before DR, but is one after.
- False Negative (FN). The point is an outlier before DR, but not after.
- True Negative (TN). The point is not an outlier before DR, nor after.

We can summarize these quantities in a *confusion matrix*, as shown in Figure 2. In an ideal scenario the confusion matrix would be diagonal (i.e. 0 FPs and FNs), indicating that all outliers and non-outliers were correctly retained by the DR-methods. However, in practise the matrix will often contain some FPs and FNs, and the performance of a DR-methods is judged by all four quantities.

		Outlier before DR?	
		Yes	No
After DR?	Yes	TP	FP
	No	FN	TN

Figure 2. Confusion matrix showing what happened to outliers after DR

Confusion matrices are used in several research communities to asses the performance of, e.g., binary classifiers and statistical tests. Often a single number is needed to capture performance, which subsequently results in a combination of the four quantities in the table. Several such combinations exist and are used in various fields of research, see the overview in paper Powers (2011).

We intend to describe three performance measures that are often used in the literature, but before we do so we highlight one complicating aspect of our problem scenario. Since we deal with outliers, most practical data sets will have a significantly larger number of non-outliers than outliers. Hence, in the confusion matrix the TN will usually be the largest number. As an example of a performance measure that is affected by this, we look at *accuracy*, defined as

$$\text{accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{FN} + \text{TN}}.$$

Since TN is dominating number, accuracy will always be close to 1, making it difficult to identify small differences in performance. Hence, the three performance measures that are described below are selected because they are capable of handling this issue.

3.2.1 F1-score

The *F1-score* is a combination of *recall* and *precision*:

- Recall. The fraction of high-dimensional outliers retained by the DR-methods (i.e. $TP/(TP + FN)$), which is maximized for $FN = 0$.
- Precision. The fraction of low-dimensional outliers that were also high-dimensional outliers (i.e. $TP/(TP + FP)$), which is maximized for $FP = 0$.

The F1-score takes the harmonic mean of precision and recall, resulting in a number between 0 (when $TP=0$) and 1 (when $FP=FN=0$):

$$\begin{aligned} F1 &= 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} \\ &= 2 \cdot \frac{TP/(TP + FP) \cdot TP/(TP + FN)}{TP/(TP + FP) + TP/(TP + FN)} \\ &= \frac{2TP}{(2TP + FN + FP)}. \end{aligned} \tag{9}$$

If $TP + FN = 0$ or $TP + FP = 0$ then the F1-score is defined as 0. Note that the element TN of the confusion table does not affect the score, and it is therefore not affected by the sparsity of outliers. The F1-score is used in, e.g., Information Retrieval [Cao et al. \(2009\)](#); [Martins et al. \(2010\)](#) and Machine Learning [Escalante \(2005\)](#); [Sha and Pereira \(2003\)](#); [Valstar et al. \(2011\)](#).

3.2.2 Matthews Correlation

The *Matthews Correlation* (due to [Matthews \(1975\)](#)) computes a correlation coefficient between the class labels (i.e. outlier or non-outlier) in high and low dimension of each point in the data sets. It results in a number between -1 (perfect anti-correlation) and 1 (perfect correlation), with 0 indicating the absence of correlation. Below we will derive an expression for the Matthews Correlation in terms of the elements of the confusion matrix. Define

$$h_i = \begin{cases} 1 & \text{if point } i \text{ is an outlier in high dimension} \\ 0 & \text{otherwise,} \end{cases}$$

and similarly

$$l_i = \begin{cases} 1 & \text{if point } i \text{ is an outlier in low dimension} \\ 0 & \text{otherwise.} \end{cases}$$

With the l_i and h_i we can compute the correlation between the class labels $l_1 \cdots l_N$ and $h_1 \cdots h_N$ (N is the total number of points in the data set). The correlation can be interpreted as a measure of how well outliers are preserved.

This correlation ρ is computed from

$$\rho = \frac{1}{N-1} \frac{\sum_{i=1}^N (l_i - \bar{l})(h_i - \bar{h})}{\sigma_l \sigma_h}$$

where

$$\bar{l} = \frac{1}{N} \sum_i l_i = \frac{\text{TP} + \text{FP}}{N}, \quad \bar{h} = \frac{1}{N} \sum_i h_i = \frac{\text{TP} + \text{FN}}{N} \quad (10)$$

using notation from the confusion matrix. The σ_l is the standard deviation of the l_i , i.e.,

$$\begin{aligned} \sigma_l &= \sqrt{\frac{1}{N-1} \sum_i (l_i - \bar{l})^2} \\ &= \sqrt{\frac{1}{N-1}} \sqrt{\sum_i (l_i^2 - 2l_i \bar{l} + \bar{l}^2)} \\ &= \sqrt{\frac{1}{N-1}} \sqrt{\sum_i (l_i - 2l_i \bar{l} + \bar{l}^2)} \\ &= \sqrt{\frac{1}{N-1}} \sqrt{N\bar{l} - 2N\bar{l}^2 + N\bar{l}^2} \\ &= \sqrt{\frac{N}{N-1}} \sqrt{\bar{l}(1-\bar{l})}. \end{aligned} \quad (11)$$

Similarly, the standard deviation of the h_i becomes $\sigma_h = \sqrt{\frac{N}{N-1}} \sqrt{\bar{h}(1-\bar{h})}$. Substituting these quantities in the correlation yields

$$\begin{aligned}
\rho &= \frac{\sum_{i=1}^N (l_i - \bar{l})(h_i - \bar{h})}{\sigma_l \sigma_h} \\
&= \frac{\sum_{i=1}^N (l_i - \bar{l})(h_i - \bar{h})}{N \sqrt{\bar{l}\bar{h}(1-\bar{l})(1-\bar{h})}} \\
&= \frac{\sum_{i=1}^N (l_i h_i - \bar{l}h_i - l_i \bar{h} + \bar{l}\bar{h})}{N \sqrt{\bar{l}\bar{h}(1-\bar{l})(1-\bar{h})}} \\
&= \frac{\sum_{i=1}^N (l_i h_i) - N\bar{l}\bar{h} - N\bar{l}\bar{h} + N\bar{l}\bar{h}}{N \sqrt{\bar{l}\bar{h}(1-\bar{l})(1-\bar{h})}} \\
&= \frac{\sum_{i=1}^N (l_i h_i) - N\bar{l}\bar{h}}{N \sqrt{\bar{l}\bar{h}(1-\bar{l})(1-\bar{h})}}.
\end{aligned} \tag{12}$$

Using $\sum_{i=1}^N (l_i h_i) = \text{TP}$ and Eq. (10), some algebra yields

$$\rho = \frac{\text{TP} \cdot \text{TN} - \text{FP} \cdot \text{FN}}{\sqrt{(\text{TP} + \text{FN})(\text{TP} + \text{FP})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}}. \tag{13}$$

If any of $\text{TP} + \text{FN}$, $\text{TP} + \text{FP}$, $\text{TN} + \text{FP}$, or $\text{TN} + \text{FN}$ are 0, then ρ is defined as 0. Note that, since ρ is a correlation, it is not affected by the large number of non-outliers.

The Matthews Correlation is often used in Bioinformatics to assess the performance of classifiers, see, e.g. [Shen and Chou \(2007\)](#); [Mondal et al. \(2006\)](#); [Kandaswamy et al. \(2012\)](#).

3.2.3 Relative Information score

The Relative Information score was proposed by [Kononenko and Bratko \(1991\)](#) and relies on ideas from the Information Theory field. In this section we derive an expression for the Relative Information score based on the confusion matrix. Suppose we consider one particular point, then a priori we can compute the probability that it is an outlier from the confusion matrix

$$\mathbb{P}(\text{outlier in high dimension}) = \frac{\text{TP} + \text{FN}}{N}.$$

After DR, we can compute this same probability for the same point as

$$\mathbb{P}(\text{outlier in low dimension} \mid \text{outlier in high dimension}) = \frac{\text{TP}}{\text{TP} + \text{FN}}.$$

[Kononenko and Bratko \(1991\)](#) argue that any well-performing classifier (DR-methods) should at least result in a confusion table with $\frac{\text{TP}}{\text{TP} + \text{FN}} > \frac{\text{TP} + \text{FN}}{N}$, otherwise it has lost information from the original data. This forms the basis for their Relative Information score.

We introduce some notation and denote by $\mathbb{P}(C_i = c)$ the probability that point i in the data set has class c , with $c = 1$ indicating that it is an outlier in high dimension, and $c = 0$ that it is a non-outlier. From the confusion matrix, we know that

$$\mathbb{P}(C_i = 1) = \frac{\text{TP} + \text{FN}}{N} \tag{14}$$

$$\mathbb{P}(C_i = 0) = \frac{\text{FP} + \text{TN}}{N}. \tag{15}$$

$$\tag{16}$$

After DR each point is again an outlier or non-outlier, but this time in low dimension. We denote the probability that point i has class c , given that it also had class c in high dimension, by $\mathbb{P}(C'_i = c \mid C_i = c)$. From the confusion matrix, we find that

$$\mathbb{P}(C'_i = 1 \mid C_i = 1) = \frac{\text{TP}}{\text{TP} + \text{FN}} \tag{17}$$

$$\mathbb{P}(C'_i = 0 \mid C_i = 0) = \frac{\text{TN}}{\text{FP} + \text{TN}}. \tag{18}$$

$$\tag{19}$$

[Kononenko and Bratko \(1991\)](#) measure the amount of information (as defined by [Shannon \(1948\)](#)) necessary to correctly classify point i as

$$-\log_2(\mathbb{P}(C'_i = c \mid C_i = c)).$$

They then give a positive score for a DR-methods that satisfies $\mathbb{P}(C'_i = c \mid C_i = c) > \mathbb{P}(C_i = c)$:

$$\log_2 (\mathbb{P}(C'_i = c|C_i = c)) - \log_2 (\mathbb{P}(C_i = c)).$$

Some algebra shows that this is indeed a positive score. If $\mathbb{P}(C'_i = c|C_i = c) < \mathbb{P}(C_i = c)$ the score is

$$\log_2 (1 - \mathbb{P}(C_i = c)) - \log_2 (1 - \mathbb{P}(C'_i = c|C_i = c)),$$

which is negative. When $\mathbb{P}(C'_i = c|C_i = c) = \mathbb{P}(C_i = c)$ the score is defined as 0. The total score I of a DR-methods is then

$$I = \sum_{i=1}^N \mathbb{1}_{\{\mathbb{P}(C'_i=c|C_i=c) > \mathbb{P}(C_i=c)\}} \cdot [\log_2 (\mathbb{P}(C'_i = c|C_i = c)) - \log_2 (\mathbb{P}(C_i = c))] \\ + \mathbb{1}_{\{\mathbb{P}(C'_i=c|C_i=c) < \mathbb{P}(C_i=c)\}} \cdot [\log_2 (1 - \mathbb{P}(C_i = c)) - \log_2 (1 - \mathbb{P}(C'_i = c|C_i = c))].$$

Usually, when comparing classifiers I is reported relative to the expected information E needed to correctly classify each point:

$$E = - \sum_{i=1}^N \mathbb{P}(C'_i = c|C_i = c) \cdot \log_2(\mathbb{P}(C'_i = c|C_i = c)). \quad (20)$$

The Relative Information score I_r is then

$$I_r = \frac{I}{E} \cdot 100\%. \quad (21)$$

Note that I_r can become negative because I can also be negative. Inserting Eqs. (14)-(18) into Eqs. (20) and (21) yields an expression in terms of the elements of the confusion matrix.

4 Data sets

In the previous sections we described setup of our experiments, the DR-techniques, and how we measure their performance. The experiments use three real-world data sets which we describe here,

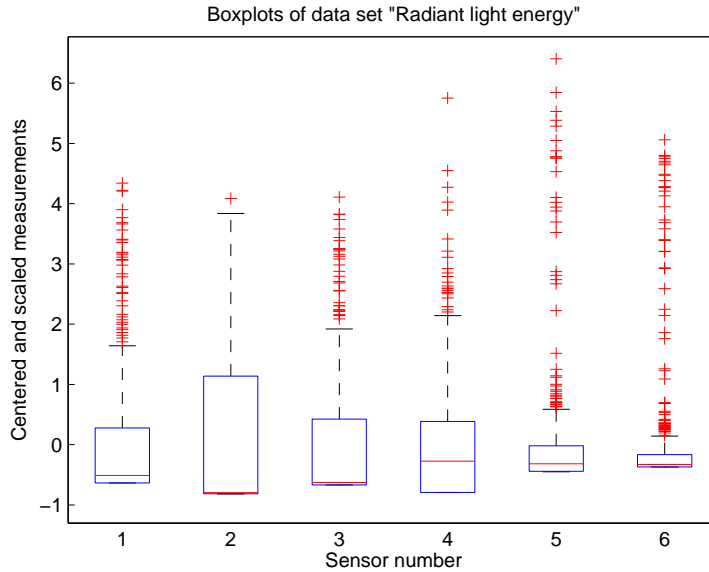


Figure 3. Boxplots of the six sensors in the “Radiant light energy” data set

4.1 Radiant light energy measurements

The measurements in this data set are from sensors deployed in several office buildings in New York City, as part of Columbia University’s EnHANTs project. The sensors measure *irradiance* (radiant light energy), and this data set contains values measured during about one year.

Figure 3 shows boxplots of each of the six sensors in this data set, with the measurements centered and scaled as discussed in Section 3. Each boxplot reflects the distribution of the 500 measurements by one sensor, and highlights possible outliers. Each sensor contains 40-60 possible outliers, except for the second sensor which has just one. The Peeling algorithm from Section 3.1 will select which of these points we will use as outliers in our experiments. Note also that the median of each sensor’s values (except sensor 4) is close to the .25 quantile, indicating that those distributions are skewed towards the smaller values.

More detailed information on the data set can be found in [Gorlatova et al. \(2011\)](#), or from the CRAWDAD website ([Gorlatova et al. \(2011\)](#)) where the data can be downloaded. For computational reasons, we do not use all the data for the experiments in this paper, but select 500 random measurements from each of the six sensors.

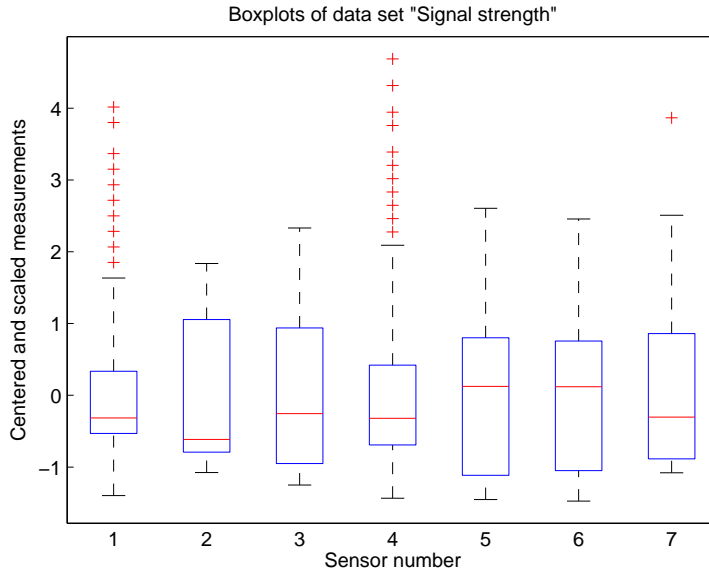


Figure 4. Boxplots of the seven sensors in the “Signal strength” data set

4.2 Signal strength data

This data originates from a WSN deployed in a library building, where sensors measure radio frequency energy level (RSSI) on all 802.15.4 channels in the 2.4 GHz ISM Band. In essence, RSSI is an indication of the power level of a signal received by the antenna on the sensor node. The building has several collocated Wi-Fi networks in normal operation that cause interference, so the WSN is used to monitor the signal strengths on one location in this Wi-Fi network. The WSN consists of 16 sensor nodes (each monitoring a single Wi-Fi channel) of which we used only 7, because the performance of convex hull algorithm in Onion Peeling decreases significantly for dimensions higher than 8 (see [Barber et al. \(1996\)](#)). Again, we took 500 randomly selected measurements of each node to form this data set.

The boxplots of the sensor values in this data set are shown in [Figure 4](#). In contrast to “Radiant light energy” data set, the measurements of the sensors in the “Signal strength” data set contain fewer possible outliers and are more evenly distributed. All possible outliers are positive values, corresponding to a strong incoming Wi-Fi signal.

More details about the data can be found in [Noda et al. \(2011\)](#), or in the CRAWDAD repository ([Noda et al. \(2012\)](#)).

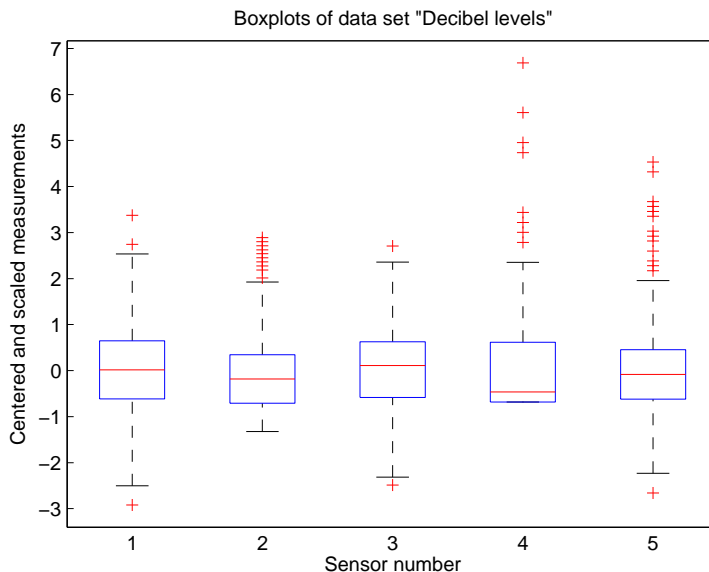


Figure 5. Boxplots of the five sensors in the “Decibel levels” data set

DR-technique	Light	Signal	Decibel
PCA	0.3333	0	0.3529
MDS	0.9091	0.8750	0.8889
t-SNE	0	0	0

Table 1. F1-score ($\in [0, 1]$) of each combination of DR-technique and data set

4.3 Decibel levels

This data set consists of five sensors nodes deployed in a kindergarten, one in each room of a single-story building, that are used to monitor the indoor climate. Among other parameters, the nodes measure decibel levels, and report these regularly to a central base station. We took 500 measurements from each sensor on a day in May 2011 and included them in this data set.

Figure 5 shows that most sensors have fairly evenly distributed values, with several outliers on both sides of the median. However, kindergartens tend to be noisy rather than quiet, so most outliers are on the positive side of the median.

DR-technique	Light	Signal	Decibel
PCA	0.3302	-0.0149	0.3477
MDS	0.9119	0.8801	0.8926
t-SNE	-0.0045	-0.0061	-0.0064

Table 2. Matthews Correlation ($\in [-1, 1]$) for each combination of DR-technique and data set

DR-technique	Light	Signal	Decibel
PCA	0.7261	-0.1295	0.6398
MDS	1.0509	0.9157	0.8971
t-SNE	-0.0404	-0.0244	-0.0226

Table 3. Relative Information Score ($\in [-\infty, \infty]$) for each combination of DR-technique and data set

5 Results and discussion

We apply the experimental setup of Section 3 to the DR-techniques of Section 2 and summarize the results in Tables 1-3. These tables contain the F1-score, Matthews Correlation, and Relative Information score for each combination of DR-technique and data set, where a high score implies that the technique preserves outliers well on that data set. The F1-scores in Table 1 show that MDS achieves the highest scores, with values more than twice as large as those of PCA on the first and third data set. The lowest possible score on all data sets is by t-SNE: an F1-score of 0. With the Matthews Correlation and Relative Information score in Tables 2 and 3 we see similar results: MDS consequently attains high scores, PCA performs reasonably well on the first and third data set, and t-SNE has overall low scores.

Since we reduce each data set to two dimensions, we can plot the resulting low-dimensional data set and inspect what happens with outliers after applying the three DR-methods. In Figures 6-8 we plot the low-dimensional version of the second data set “Signal strength” (in circles), with outliers in the original high-dimensional data set marked with a triangle. Figure 6 shows that several of the outliers are mapped to the interior of the reduced data set by PCA. In contrast, the low-dimensional data set created by MDS shows all high-dimensional outliers close to the boundary. Lastly, t-SNE maps all outliers to the interior of the low-dimensional data set, which illustrates its low scores.

By analysing the objective of the three DR-techniques, we can explain the observed differences in performance. Firstly, PCA is a technique that focuses on preserving variance, so it will only preserve outliers if they happen to be in a direction of high variance. Figure 1 from the introduction provides another

illustration of what can happen to an outlier that is in a direction with low variance. The figure corresponds to reducing a two-dimensional data set to one dimension (the line) with PCA, and clearly shows how the top-left outlier ends up in the center of the reduced data set.

MDS optimizes the squared stress optimization criterion in Eq. (4), which includes the term $\|\mathbf{x}_i - \mathbf{x}_j\|_M$. This term is the distance between two points \mathbf{x}_i and \mathbf{x}_j , which is typically very large when one of the points is an outlier. The criterion uses these distances to the power 4, so the outliers have a large effect on the squared stress criterion. Hence, minimizing these distances has a massive positive effect when on this criterion and thus MDS preserves outliers well.

t-SNE optimizes the Kullback-Leibler divergence (8), which attaches high costs to nearby points in high dimensional space (large p_{ij}) that are mapped to far away points in low dimensional space (small q_{ij}). Hence, nearby points in high dimensional space are kept nearby in low dimensional space. This does not hold for points that are far away in high dimensional space – outliers, which have low p_{ij} – as they are mapped to nearby points (with high q_{ij}) with very low costs. So t-SNE tries to keep nearby points nearby and is therefore more suitable for preserving clusters than for preserving outliers.

Also, t-SNE has some computational complexities. The Kullback-Leibler divergence in Eq. (8) is a non-linear function of the low-dimensional points \mathbf{y}_i and can have several local minimums. Minimizing Eq. (8) is done by choosing a random starting point for the \mathbf{y}_i , followed by a number of optimization steps using, e.g., a Gradient Descent approach. The optimization stops when it reaches a (possibly local) minimum, and returns its latest values for the \mathbf{y}_i . Hence, the low-dimensional points depend on the starting point chosen for the optimization algorithm, and thus its performance with respect to outlier preservation also depend on the starting values of the \mathbf{y}_i . The last rows of Tables 1-3 show the score for one particular starting point, but we repeated the experiments with t-SNE for various starting points. We discovered no correlation between the minimized value of the Kullback-Leibler divergence and the achieved performance score, so the results reported in Tables 1-3 are representative for the performance of t-SNE.

From the analysis above we see that from the three selected methods, MDS achieves the highest scores and is best capable of preserving outliers. However, it is not necessarily the best DR-technique available, since many others exist in literature. In particular, the class of *supervised* DR-techniques (PCA, MDS, t-SNE are unsupervised) might provide methods with better performance than MDS. These techniques aim to reduce dimensionality while simultaneously trying to retain “sufficient information” for a classification task (which, in our case, would be retaining outliers). Hence, they could be applied to the scenario in this paper, and possibly have good performance. Nevertheless, supervised DR-techniques are not included here, because we assume that the DR-techniques

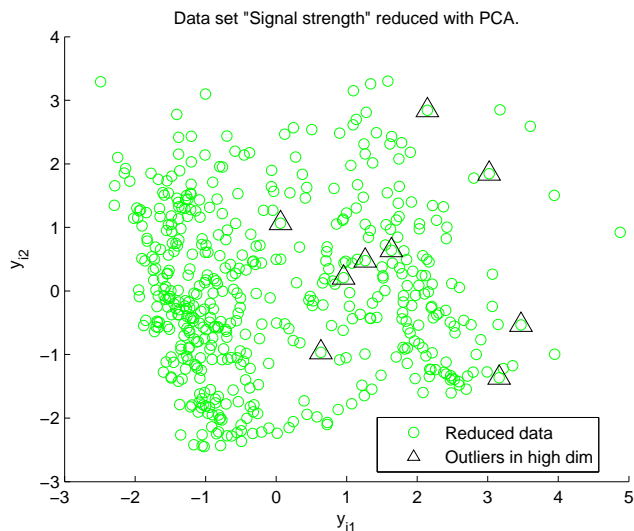


Figure 6. Data set “Decibel levels” after dimensionality reduction with PCA (circles). The triangles mark the outliers that were found in the original high-dimensional data set

have no apriori knowledge about the outliers, and thus they are not suitable for this paper. Readers interested in supervised DR-techniques are referred to, e.g., [Shyr et al. \(2010\)](#).

The performance measures in this paper are all based on the elements of the confusion matrix, which do not contain information about whether a point is a ‘large’ or ‘small’ outlier. Hence, with these scores we will not be able to, e.g., find out which outlier has the large affect on a score. This ‘binary’ view of an outlier is, however, important for the scenario in the current paper. Our motivation comes from applications where it is of critical importance to correctly identify an outlier after DR. If an outlier is no longer an outlier after DR, then it is useless for the application. Nevertheless, if this ‘binary’ approach can be relaxed from the point of view of the application, other scores might be more appropriate (see, e.g., [Bradley \(1997\)](#)).

6 Conclusions and recommendations

In this paper we described three well-known Dimensionality Reduction techniques (Principal Component Analysis, Multidimensional Scaling, and t-Stochastic Neighbourhood Embedding) and analysed how well they are capable of preserving outliers. Based on three different scores (F1-score, Matthews Correlation,

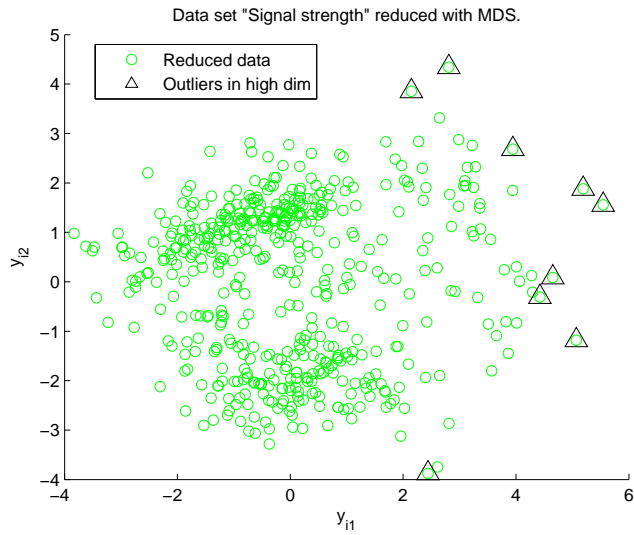


Figure 7. Data set “Decibel levels” after dimensionality reduction with MDS (circles). The triangles mark the outliers that were found in the original high-dimensional data set

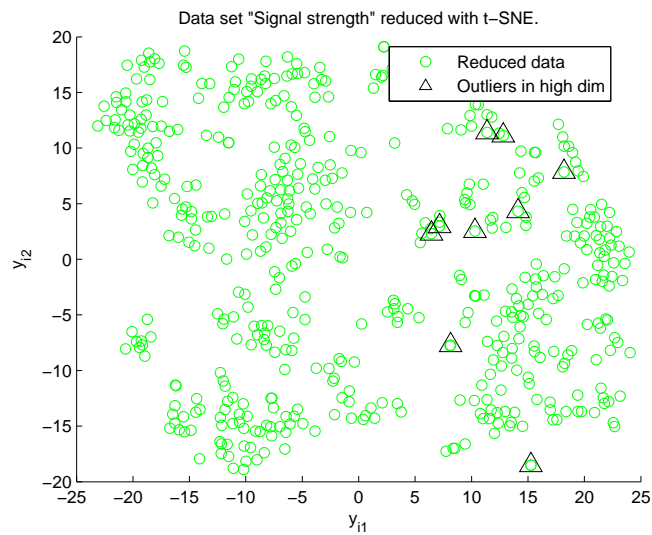


Figure 8. Data set “Decibel levels” after dimensionality reduction with t-SNE (circles). The triangles mark the outliers that were found in the original high-dimensional data set

and Relative Information score), and using three real-world data sets, we assessed the performance of each method on each data set.

The resulting analysis shows that, among the three described DR-methods, Multidimensional Scaling is best at preserving outliers. It consequently achieves the highest scores, and performs significantly better than both Principal Component Analysis and t-Stochastic Neighbourhood Embedding. In the discussion, we explain that this difference in performance is caused by the specific objectives of the techniques: PCA tries to preserve variance, MDS preserves large distances (i.e. outliers), and t-SNE preserves clusters. In general, we recommend that the dimensionality reduction technique is chosen with the intended application in mind. For outlier detection MDS is a good choice, for preserving variance PCA is the best choice, and for preserving clusters t-SNE is a good choice.

Future research includes investigating specific types of Dimensionality Reduction (e.g. supervised DR-methods, real-time DR-methods), and how they are affected by outliers.

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