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RESEARCH ARTICLE

Outlier detection in UV/Vis spectrophotometric data

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ABSTRACT

UV/Vis spectrophotometers have been used to monitor water quality since the early 2000s. Calibration of these devices requires sampling campaigns to elaborate relations between recorded spectra and measured concentrations. In order to build robust calibration data sets, several spectra must be recorded per sample. This study compares two approaches – principal component analysis and data depth theory – to identify outliers and select the most representative spectrum (MRS) among the repetitively recorded spectra. Detection of samples that contain outliers is consistent between the methods in more than 70% of the samples. Identification of spectra as outliers is consistent in more than 95% of the cases. The identification of MRS differs depending on the approach used. In their current form, both of the proposed approaches can be used for outlier detection and identification. Further studies are suggested to combine the methods and develop an automated ranking and sorting system.

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KEYWORDS
UV/Vis spectrophotometer; outlier; identification; sample; calibration

1. Introduction

For two decades, researchers and practitioners have been using UV/Vis spectrophotometers to estimate concentrations in water matrices: TSS, total COD, NO_2, etc. are estimated from absorbances at several wavelengths. (Rieger *et al.* 2004). The accuracy and robustness require a local calibration (Langergraber *et al.* 2003, 2004a, 2004b, Torres and Bertrand-Krajewski 2008). Taking into account the local specifications of the water matrices, samples are collected, measured with the spectral device and concentrations are measured with laboratory analysis. In addition to the existing global calibrations (non-specific), local calibrations can be classified into two categories: (i) 'concentration–concentration' based on the concentrations estimated by the sensor and a calibration furnished by the manufacturer (often referred to as 'global calibration' e.g. in Caradot *et al.* 2015), (ii) 'spectrum–concentration' based on the spectral data, without using the global calibration. Among all the existing methods, partial least squares, support vector machine and polynomial regression are the most popular methods to calibrate such a probe. During the construction of the calibration data-set, several spectra can be recorded for the same water sample. The work presented in this paper investigates new methods that can be used as a preliminary step for the second type of local calibration, for which repetitions of spectral measurements have been performed. Calibration functions are normally derived from data sets containing one single spectrum per sample, sometimes while taking into account uncertainties on one (Rieger *et al.* 2006) or both data (Lepot *et al.* 2013). Some researchers have also studied outlier detection in such large data sets (López-Kleine and Torres 2014, Zamora and Torres 2014). However, when several spectra are recorded per sample (e.g. one spectrum can be recorded every 15 s), this advancement raises some new questions: Do the recorded repetitive spectra contain outliers? How can these outliers be identified? How can a representative spectrum be selected? To our knowledge, no previous studies have addressed this subject related to wastewater in this manner. In this study, two methods are presented and tested on two different data sets.

2. Data sets and methods

In this section, we introduce the two data sets and the two methods – principal component analysis (PCA) and data depth theory (DDT).

2.1. Data sets

The two data sets have been collected in two different locations and from two different wastewaters. They are referred to as the WWTP data-set and the Zürich data sets, respectively. The latter is further divided into four smaller data sets: FD, FU, UD, UU.

2.1.1. WWTP inlet data-set

Wastewater samples were collected at the intake of the Fontaines-sur-Saône WWTP in France (30,000 inhabitants, combined sewer), during four dry-weather non-consecutive days in 2011. For each sample, two kinds of data were recorded: (i) from 15 to 25 spectra (every 15 s), and (ii) concentrations obtained by triplicate standard laboratory analyses for TSS, total, and dissolved COD. The submersible, in situ spectrophotometer used

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in this study was a spectro::lyser with an optical path length of 2 mm, a wavelength step of 2.5 nm (221 values per spectrum), recording UV/Vis spectra 200–750 nm (s::can Messtechnik GmbH, Vienna, Austria). The time step was the minimal 15 s between two recordings and the internal smoothing algorithm was disabled. During measurement, each of the 94 1 L samples were placed on a magnetic stirrer (rotation of 800 tr/min) and pumped in a closed circuit with a peristaltic pump.

2.2.2. Zürich data sets

A pilot-scale nitrification MBBR is operated at Eawag (Switzerland), treating source-separated urine with the aim of producing a fertilizer (Fumasoli *et al*. 2016). Thirty 3 L samples were collected during 10 weeks in 2014 to study the effects of filtration and saturation on nitrite estimation (Mašić *et al*. 2015, data published as supplementary material). Addition of nitrite/nitrate stock solutions increased the range of concentrations. Each sample was subjected to combinations of pre-treatments [(Un)-Filtered/(Un)-Diluted], resulting in four sample groups: FD, FU, UD, UU. Filtration was performed with a 0.7 µm glass fiber filter (MN GF-1, MACHEREY-NAGEL AG, Oensingen, Switzerland) and 1:10 dilution with nanopure water. The spectral device was a spectro::lyser (s::can Messtechnik GmbH, Vienna, Austria), with a path length of 0.5 mm, recording in the UV spectrum (220–399 nm) with a resolution of 1 nm and a recording time of 1 spectrum/minute. During recording, the vessel was placed on a magnetic stirrer (rotation 1000 rpm). For each sample, five spectra (one per minute) were recorded and the ammonium, nitrite, and nitrate concentrations were measured (LCK303, LCK340, LCK341, LCK342, Hach-Lange GmbH, Germany).

2.2. Methods

2.2.1. Data depth theory

Step 1: outlier removal. Let x be defined as the matrix of size $N_T \times n_x$, containing N_T recorded spectra for one sample. Each spectrum measures n_x wavelengths. Among the N_T spectra available, one or several outliers must be removed, described by Equations (1a) and (1b) (Lepot 2012):

$$ED_j = \frac{1}{N_T}\sqrt{\sum_{i=1}^{n_x}\left(Abs_{j,i} - Abs_{k\neq j,i}\right)^2} \tag{1a}$$

$$ED_j > k_M \times median\left(\left[ED_1 : ED_{N_T}\right]\right) \tag{1b}$$

where ED_j is the Euclidean distance of spectrum j, $Abs_{j,i}$ is the absorbance (m^{-1}) of wavelength i for spectrum j, and k_M is a multiplicative coefficient. If a spectrum has a Euclidean distance higher than k_M times the median of the N_T spectra (Equation (1b)), it will be considered an outlier. This method is sensitive to the subjective value of k_M. For the remainder of this manuscript, the method is referred to as DDT_ED_1, DDT_ED_2, and DDT_ED_3, depending on the value of k_M.

In order to increase the objectivity and the robustness of the method previously used in Lepot (2012), it is expanded with additional steps based on data depth theory (e.g. in López-Pintado and Romo 2006) and is referred to as DDT_DDT.

At the end of the first step (Equations (1a) and (1b)), N_R spectra are retained among the N_T initially available. For every spectrum j, absorbances $Abs_{j,i}$ are compared to $Abs_{k,i}$ (with $k \neq j$) for each wavelength i. If for all the n_x wavelengths, the absorbances of spectrum j are lower or higher than all the other absorbances, it is considered an outlier.

Step 2: identification of the most representative spectrum. For each spectrum j among the N_R retained spectra and for each wavelength i, the relative position of the spectrum is studied by comparison to all other spectra k, and summarized as follows (Figure 1):

- Comparison of absorbances:
- For each wavelength i, the spectra with a higher/equal/lower absorbance than in spectrum j are counted and stored in vector $L_1/L_2/L_3$. Vector L_2 is also referred to as *Equal*.
- The difference between the number of higher and lower absorbances is stored in the vector *Diff*, i.e. $Diff = |L_1 - L_3|$.

This procedure is repeated for every wavelength i and every retained spectrum j to create the matrices *DIFF* and *EQUAL*. The matrices are summed over the wavelengths into the column vectors S_{DIFF} and S_{EQUAL} (Figure 1). In order to identify the MRS, here defined as 'the most in the middle', the selected spectrum R is identified by the minimum in S_{DIFF} and, if several spectra offer the same minimum, the one that maximizes S_{EQUAL}.

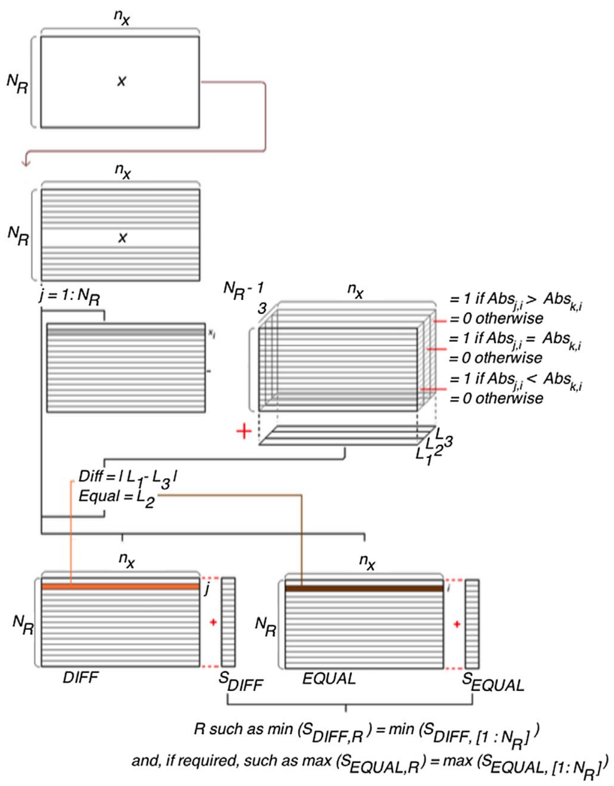

Figure 1. Scheme of the method Step 2: DDT for the identification of the MRS, applied in DDT_ED_k_M and DDT_DDT.

2.2.2. PCA

This method relies on the scores of the first principal component in PCA (Jolliffe 2002, Mašić *et al.* 2015). As before, let x denote the matrix containing N_T recorded spectra for one sample. Each spectrum measures n_x wavelengths. In other words, we have N_T observations and n_x variables.

Step 1: mean-centering. Data preprocessing is performed by centering the data in a column-wise manner around the mean vector $\bar{x}$ $(1 \times n_x)$:

$$x_{MC} = x - \bar{x} \tag{3}$$

where x_{MC} is the mean-centered matrix.

Step 2: singular-value decomposition. The principal component loading vectors are obtained by singular-value decomposition:

$$x_{MC} = USV^T \tag{4}$$

S the diagonal matrix $(N_T \times n_x)$, U the unitary matrix $(N_T \times N_T)$, V^T the transpose of V $(n_x \times n_x)$ whose column vectors are the principal component loading vectors.

Step 3: score matrix. The score matrix T $(N_T \times n_x)$ is obtained by

$$T = x_{MC}V. \tag{5}$$

Finally, the first column in T corresponds to the scores for the first principal component (PC1) and this column vector is selected for further analysis. Each spectrum has one PC1 score.

The PCA Expert method involves a visual inspection of the PC1 scores. This method relies on the subjective interpretation by an expert, who determines how distant the scores are compared to the remaining scores in the same sample.

PCA_2 relies on automated selection, based on the mean and standard deviation of the PC1 scores for a given sample. A spectrum is considered an outlier if its PC1 score is outside of the mean ± two standard deviations. This method also allows selecting the most representative spectrum as the one with the smallest distance between its PC1 score and the median.

3. Results and discussion

In this section, we first show a typical spectrum and discuss differences and similarities. Then, the two methods are compared for each of the two data sets. The detailed results are fully presented in five tables in Appendix A, following the frame shown in Table 1.

3.1. Typical absorbance spectra

The appearance of a spectral absorbance curve depends on the compounds and their concentrations in the sample and whether and to what extent they absorb light in the studied wavelength range. In the Zürich data, the samples consist of source-separated urine with added nitrite/nitrate stock solutions. They absorb in two wavelength ranges: very strongly around 220 nm and weakly around 300–350 nm. Figure 2 (left) shows a typical set of spectra with the absorbance plotted as a function of the wavelength. It is easily seen that there is a very strong absorbance around 220–240 nm (Mašić *et al.* 2015). The WWTP samples, on the other hand, were collected in wastewater during dry weather conditions. Figure 2 (right) shows seven spectral repetitions in one sample. By comparison, these spectra show a continuous decrease in absorbances from the UV to the visible part of the range.

3.2. Outlier detection and identification

3.2.1. Samples containing outliers

The confusion matrices in Table B.1 summarize the performance of the methods in terms of detection of outliers and consistencies of detection. Methods identify samples containing outliers in a consistent way if the number of True Positive (TP) and True Negative (TN) identifications is equal or close to the number of samples in the data-set. False detections (FP, FN) highlight inconsistencies between the methods.

The identification of samples containing outliers with DDT_ED_k_M is clearly sensitive to the k_M coefficient. By construction, DDT_ED_1 identifies outliers in each sample (TN and FP are always equal to 0). Consistencies in sample detection with DDT_ED_k_M changes slightly with the wastewater matrices: DDT_ED_2 is more consistent with DDT_ED_1 than with DDT_ED_3 for the WWTP samples; it is the opposite for the urine samples. This can likely be explained by the difference in the number of spectra per sample (up to 25 for the WWTP data-set, only 5 for the urine data sets). DDT_ED_2 appears to be a good trade-off.

For the WWTP data, DDT_DDT identifies fewer samples with outliers than DDT_ED_k_M: 39 instead of 69 for DDT_ED_3. Figure 3 (left) shows a straightforward identification of an outlier. In sample 2-WWTP, spectrum 1 is always above the other spectra in the sample. On the other hand, the method does not identify any outliers for the Zürich data. Figure 3 (right) illustrates the sensitivity to noise (the spectra are not smooth in this part) in some parts of the spectra in the FD data-set: one spectrum is clearly below the others for wavelengths lower than 250 nm. Above this, the spectrum mixes with the rest of the spectra and, thus, cannot be detected by DDT_DDT. Possibly the wastewater matrix (urine) or technical limitations of the material may explain the noise. In order to solve this problem, two subjective steps could be added to DDT_DDT: i) smoothing the spectra or ii) considering the spectrum as an outlier only if more than a certain percentage (e.g. 90%) of its values are higher or lower than the values of all other spectra. These options have not been tested in this study.

PCA_2 is also unable to detect outliers for the Zürich data: the estimation of the standard deviation (on the five spectra recorded per sample) is too influenced by any existing outliers. For data sets containing more spectra per sample, this method provides consistently detected samples in about 71% of the tested samples. This consistency ratio, defined as the ratio of true detections over the number of samples, is only of 54% for DDT_DDT.

In every data-set, PCA_Expert provides a consistent list of samples containing outliers: for the WWTP samples, at least 78% of the detection is consistent with other methods (except DDT_DDT) and 73% for the Zürich samples (except DDT_ED_1, too selective). Figure 4 (top) shows an example of sample number 7-WWTP, indicating the spectra identified as outliers by PCA_Expert and PCA_2.

3.2.2. Identification of the outliers

For a given sample containing outliers, this step ensures that the identified outlier spectrum is consistent between the methods.

Table 1. Table structure. Statistical summary: N_{SWO} is the number of samples with outlier, also converted in percentage P_{SWO}. Detailed results: S index of the sample, R index of the MRS, and the index list of the N detected outliers $O_1,\ldots,O_N$ (–, if no outlier has been detected). MRS is not determined with PCA_Expert.

Sample number	Data depth theory								PCA			
	DDT_ED_1		DDT_ED_2		DDT_ED_3		DDT_DDT		PCA_Expert		PCA_2	
	N_{SWO} (P_{SWO} %)		N_{SWO} (P_{SWO} %)		N_{SWO} (P_{SWO} %)		N_{SWO} (P_{SWO} %)		N_{SWO} (P_{SWO} %)		N_{SWO} (P_{SWO} %)	
	MRS	Outlier (s)	MRS	Outlier (s)	MRS	Outlier (s)	MRS	Outlier (s)	MRS	Outliers (s)	MRS	Outlier (s)
S	R	$O_1,\ldots O_N$	R	$O_1,\ldots O_N$	R	$O_1,\ldots O_N$	R	$O_1,\ldots O_N$	–	$O_1,\ldots O_N$	R	$O_1,\ldots O_N$

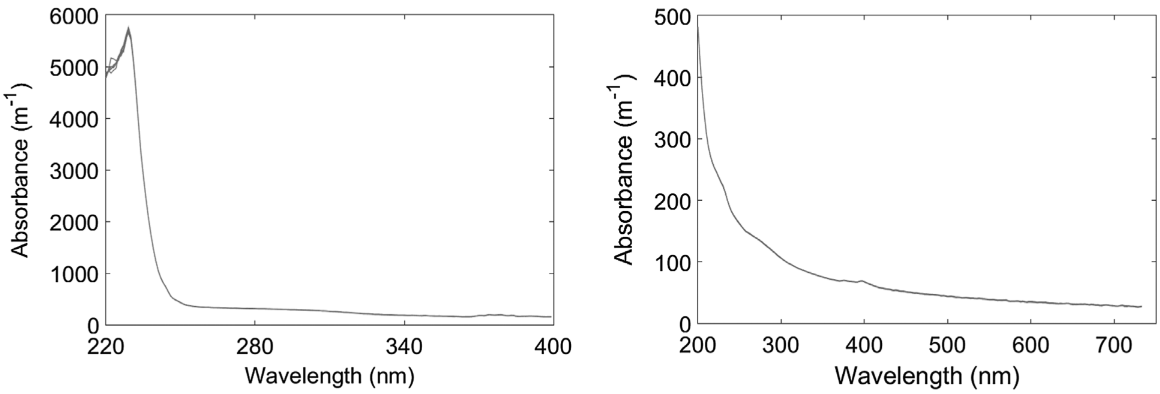

Figure 2. Typical absorbance spectra from the Zürich data-set (left) and the WWTP data-set (right), containing 5, respectively 7, spectral recordings.

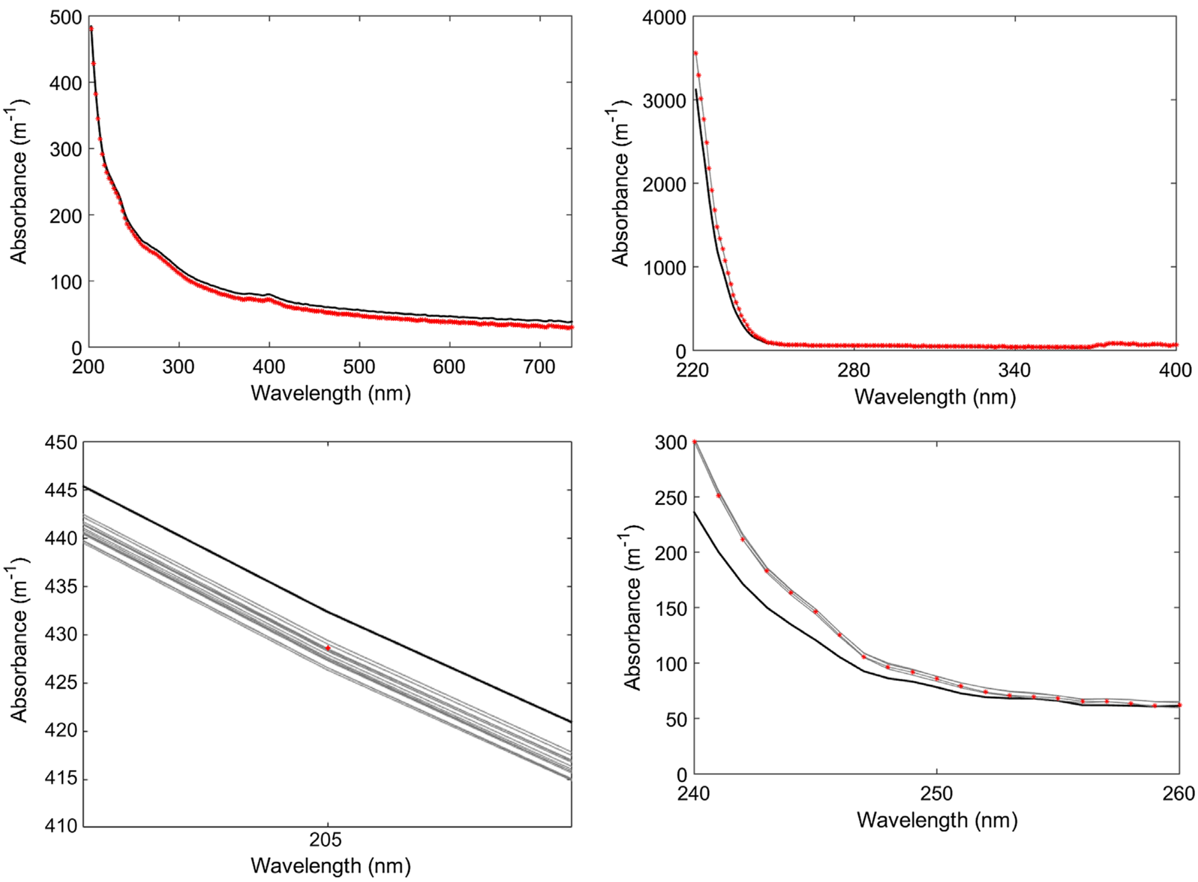

Figure 3. (left) Absorbance spectra for sample 2-WWTP, showing an ideal case with a clearly separated outlier spectrum (number 1), shown in full (top) and close-up (bottom). (right) Absorbance spectra for sample 23-FD indicating some unusual behavior. Spectra shown in gray, MRS in red markers, the outlier in black.

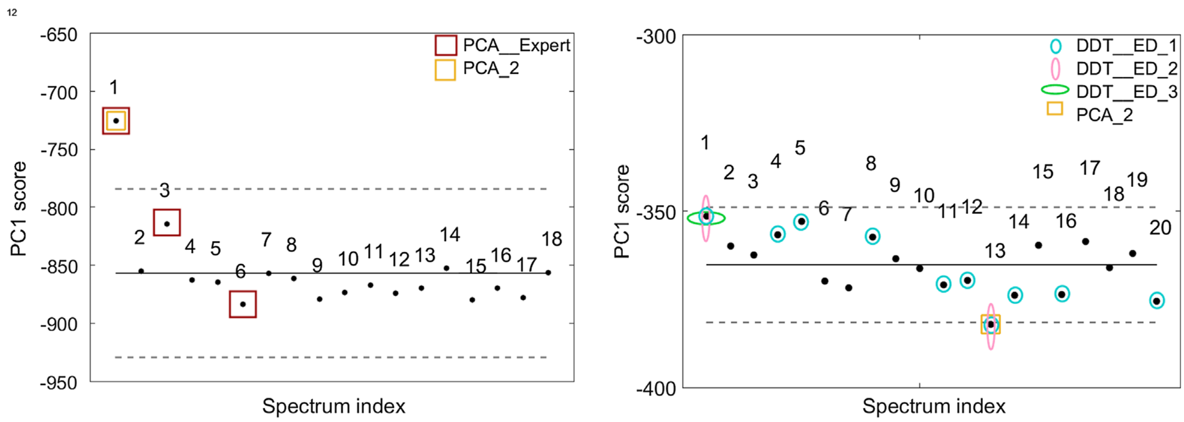

Figure 4. (left) Absorbance spectra, (right) PC1 scores. (top) sample 7-WWTP, (bottom) sample 33-WWTP. The mean with the standard deviation band is indicated on the right. (top) Spectrum 1 identified as an outlier by PCA_Expert and PCA_2 (black solid); spectra 3 and 6 by PCA_Expert (black dashed). (bottom) Inconsistent identification: spectrum 1 (black dashed) identified by DDT_ED_k_M but not by DDT_DDT or PCA-based methods. Spectrum 13 (black solid) identified only by DDT_ED_1, DDT_ED_2, and PCA_2. The MRS is plotted with the red stars.

The identified outliers are often the same (see Appendix A). Table B.2 summarizes the results in outlier identifications with a consistency ratio calculated as follows: for all the N_A samples where both methods found outliers, only N_O of them have at least one outlier O_i in common, the ratio is equal to N_O/N_A.

In order to illustrate the construction of Table B.2, one calculation is detailed. For the UD data, the consistency ratio between DDT_ED_1 and PCA_Expert is equal to 0.5. From the detailed results (Table A.4), two samples contain outliers according to both methods: $N_A = 2$ (samples 5 and 21). For sample 21, spectrum 1 is considered as outlier by both methods ($N_O = 1$). The outliers identified in sample 5 differ between the methods: spectrum 1 for DDT_ED_1 and spectra 2 and 4 for PCA_Expert (N_O does not change). Hence, the ratio is $N_O/N_A = 1/2 = 0.5$.

For the Zürich data, the consistency ratios are mostly equal to 1. For WWTP, the ratios are close to 1, except for one or two samples, where the methods identify at least one spectrum in common as outlier. Figure 3 (top left) presents consistent outlier detection between DDT_ED_3, DDT_DDT, and PCA_2. It illustrates an ideal case: one spectrum is far away and always above the other 15 spectra. This spectrum is easily identified by all the tested methods. In some rare cases, outlier identification can be inconsistent (Figures 4 (bottom) and 5).

Figure 5 shows an example of outlier detection and identification where the methods are mutually not entirely consistent. The PC1 scores are shown for sample 15-WWTP. The most sensitive method is DDT_ED_1, identifying 8/14 spectra as outliers. DDT_ED_2 and PCA_Expert identify three outliers each, but not the same ones: spectra 2 and 3 are identified by both methods, spectrum 1 by DDT_ED_2, and spectrum 8 by PCA_Expert. Neither DDT_DDT nor PCA_2 identify any outliers in this sample. A lot of variation can be observed in the PC1 scores in this sample, with possible other factors affecting the scores, such as non-homogeneous mixing.

In some cases, the methods are inconsistent due to completely unpredictable factors. For example, in sample 10-UU, PCA_Expert identifies the entire set as being outliers. None of the other methods, except the very sensitive DDT_ED_1, identifies any outliers at all. In this case, the spectra are determined as outliers by the

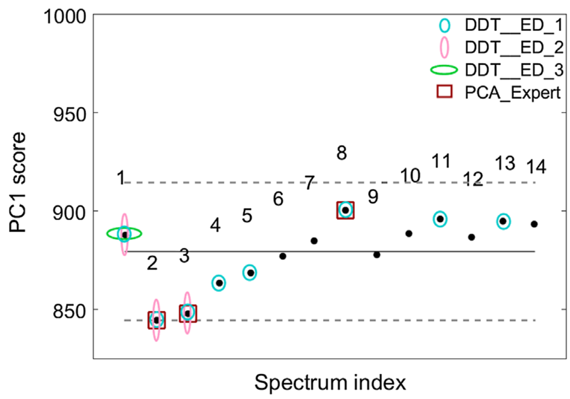

Figure 5. PC1 scores of sample 15-WWTP, with the mean and standard deviation band indicated with lines.

expert due to inconsistent absorbances when compared to the rest of the samples in this set. Sample 10-UU was disqualified due to incorrect sample preparation. Such occurrences show the limitations of the methods presented in this paper.

Figure 4 (bottom) illustrates another inconsistent outlier identification: one spectrum can be easily identified as an outlier by DDT_ED_k_M due to its distance to the other ones. DDT_DDT could not identify this spectrum because the absorbance of this spectrum is not consistently higher than those of others (e.g. the spectrum crosses the other ones at 710–720 nm).

3.3. Identification of the most representative spectra

After removing detected outliers, the MRS can be identified among the retained spectra, summarized in Table B.3.

By design, DDT_ED_k_M and DDT_DDT use the same algorithm to identify the MRS. Despite that, the consistency ratios in the identification are quite low: less than 50% in some cases for DDT_ED_1. This can be explained by the previously removed outliers. Between the methods based on DDT (DDT_ED_1 excluded), the MRS identification is more consistent for the UD and UU data than for the WWTP, FD and FU data.

The identification of the MRS via the median of the PCA scores is inconsistent with DDT based methods. In order to test whether this is caused by removal of different outliers, the identification was repeated on the WWTP data where outliers only detected by PCA_2 were removed, thus applying the methods on the same data. Results showed a consistency ratio of 28% (27 samples have the same MRS, data not shown), slightly more than in Table B.3. The differences between the methods cannot be explained by the prior outlier removal: the two approaches are clearly inconsistent.

3.4. Limitations of the study

This study is limited in some aspects. Most importantly, there is no well-defined reference to which the different methods can be compared. Detection and identification of outliers can only be compared between the methods, unless the outliers have been intentionally produced and are known in advance. Moreover, the collection of the data has been performed in two ways on two different data types. The difference in the number of recorded spectra per sample not only complicates the comparison between the methods, but most likely also affects the sensitivity of the methods to possible outliers. On the other hand, the two data sets could be seen as a realistic way of testing the two approaches on different types of data.

The Zürich data was specifically collected to study the effects of filtration and saturation. This may have introduced some additional noise due to the very high absorbances in some parts of the spectrum. Lastly, the method that measures consistency in outlier identification only compares the spectra which have been identified by both approaches, not the number of spectra in total. The obtained consistency values can thus be slightly misleading and must be used with the information obtained in the outlier detection comparison.

3.5. Perspectives

The study should be repeated on other data sets with addition of artificial outliers for easier comparison. Methods based on the dynamics of the spectra can be tested: for example, DDT_ED_k_M can be applied on the first derivative rather than on the absorbance itself. Shape recognition may as well offer some possibilities (Villez and Habermacher 2016). Outlier detection is still a delicate research issue due to the lack of a generally accepted method. With proper records (data and laboratory book i.e. logbook) outliers can be suspected and identified based on serious reasons but the truth is still unknown. The automatic outlier detection methods are based on scientific expertise. They should be updated with new knowledge and detection should be considered as partially subjective.

4. Conclusions

The work in this study focuses on repetitive spectra in wastewater samples and is not intended to be a general outlier detection method. To our knowledge, this is the first study on outlier detection in these types of samples.

The need for repeated measurements, i.e. several spectra per sample, clearly appears in the calibration of spectrophotometric devices, in order to reduce bias and the influence of errors and/or estimate the measuring uncertainties. Two different approaches (DDT and PCA) have been investigated in this study and the results allow us to reach the following conclusions:

- The different methods are consistent in detecting samples that contain outliers in 75% of the cases (average among all the methods).
- The identification of spectra as outliers is consistent between the approaches in most cases (average consistency ratio of 95%).
- The consistency between the approaches allows the user to choose which method to apply based on subjective preferences.
- For the MRS identification, the choice of method should rely on convenience (*e.g.* use the same method as for the outlier detection), since consistency is only 28%.
- The presented methods, except for the PCA_Expert, are suitable for intra- but not inter-outlier detection.

These results are promising for a systematic detection and identification of outliers in repetitive spectral recordings from wastewater samples. The tested methods are easy, do not require much computational time, and identify outlier spectra consistently for each sample. However, some weaknesses exist: DDT_ED_1 is too sensitive, PCA_2 requires more than five spectra per sample to be effective, DDT_DDT is too sensitive to noise, and PCA_Expert is subjective because it requires human expertise. The two approaches developed and tested for MRS identification are clearly inconsistent, even when applied to the same group of retained spectra.

The recommendations for potential future users can be summarized in a few key points. Automated PCA methods do not seem to be suitable when only a few spectra have been recorded per sample. When samples are collected for a specific purpose (component) and/or when the conditions can be controlled, the proposed methods should be tested while creating artificial outliers. For such cases, DDT_DDT can be applied to a selected part of the spectrum where the effects of the components are visible. If any method appears to be better than the other, a ranking and sorting system can be introduced, in which a spectrum will be considered an outlier if a certain number of the methods identify it as an outlier.

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Disclosure statement

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Appendix A: Outlier detection, identification, and retained spectrum for every sample

The appendix presents all the results for every sample of each data set, based on the frame presented in Table 1. Table A1 is for the WWTP data set, Tables A2 to A5 are for the urine data sets.

Table A.1. WWTP data set.

	Data depth theory								PCA			
	DDT_ED_1 94 (100 %)		DDT_ED_2 89 (95 %)		DDT_ED_3 69 (73 %)		DDT_DDT 39 (41 %)		PCA_Expert 82 (87 %)		PCA_2 60 (64 %)	
Sample number	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outliers(s)	MRS	Outlier(s)
1	4	1,3,6	4	--	4	--	4	--		--	3	--
2	11	1,2,3,8,11,12,13,16	15	1	15	1	15	1		1	7	1
3	5	1,2,4,6	3	1	9	--	9	--		1	9	--
4	5	1,2,3	5	2,3	4	3	4	3		3	4	--
5	5	4,6,8,9,11,13	7	6,8,13	5	6	5	6		6,8,13	5	--
6	14	2,3,4,6,7,13,15	11	7	11	7	10	5,6,7,8		4,5,6,7,8,13,15	11	7
7	18	1,3,6,9,10,12,15	11	1,3	11	1	11	1,3		1,3,6	5	1
8	4	1,3,7,8,9	4	1	4	--	4	--		--	2	--
9	3	1,2,5,6,7,9	11	5,6,7	11	--	11	--		--	3	--
10	9	1,2,4,5,6,11,13,16	8	1	8	1	8	1		1	7	1
11	13	1,2,4,6,10,12,15	13	1	13	--	13	--		--	2	--
12	1	3,4,6,10,11,12	8	11	8	11	1	--		3,10,11,12	1	11
13	14	1,3,8,9,10,11,12,15	14	8,10	14	--	14	--		3,8,10,15	17	8
14	5	1,2,7,9,10,12	8	1,2, 9	5	--	5	--		1,2,9,12	5	--
15	10	1,2,3,4,5,8,11,13	12	1,2,3	10	1	12	--		2,3,8	12	--
16	13	1,2,4,5,7,9	6	4	6	4	6	--		1,2,4,7	12	4
17	5	1,3,6,8,10,11	2	1	2	1	2	--		1,6	5	1
18	6	1,2,3,5,8,10,12	6	--	6	--	6	--		13	6	--
19	7	1,2,5,8,10,12	7	1,12	7	1,12	7	--		1,2,12	4	--
20	7	1,5,6,8,9,10	3	8,9	3	9	11	--		8,9	4	--
21	10	1,4,5,9,11,12	3	1	3	1	3	1		1,11,12	10	1
22	10	1,2,6,8,11,12	10	1,6,11	10	11	10	--		1,6,11,12	7	--
23	11	1,2,3,4,8,9	11	1,4	11	4	7	--		1,4	7	4
24	8	1,2,3,6,10,12	7	--	7	--	7	--		2,10	4	--
25	10	1,3,6,7,9,13	10	7,9	10	--	10	--		3,7,9	12	--
26	22	1,2,3,4,5,7,9,10,15,16,20,24,25	11	1,15	11	15	11	15		1,4,15,25	26	15
27	10	1,2,3,4,5,12	10	3,12	10	3,12	10	12		3,12	6	12
28	8	1,2,3,4,7,11	8	1	8	1	6	1,2		1,2,11	5	1
29	10	1,2,3,4,6,7,8	15	1,2,8	15	2	14	--		1,2	14	--
30	6	1,2,7,8,10,12,14	6	1,8,14	6	--	6	8		14	5	--
31	14	1,2,3,4,5,8,12,16	7	1,2,8,16	15	1,16	9	2		1,16	7	1,16
32	5	1,2,3,6,8,12,13,16	10	1,8	10	1	10	1		1,2,8	10	1
33	9	1,4,5,8,11,12,13,14,16,20	9	1,13	10	1	9	--		--	9	13
34	15	1,2,3,4,7,9,14	6	7	6	--	6	--		--	6	--
35	16	1,2,4,5,10,11,12,14	16	4,5, 14	3	14	16	--		--	3	14
36	11	2,3,4,5,8,10,12,13,20,22,23,24,25	26	4,12,13	26	4	26	4		1,2,4,8,9,10,12,13	18	4
37	7	4,6,9,10,12,13	3	6	3	6	3	6		6	2	6
38	8	2,4,6,7,11,13,14,15,18	8	7	8	7	8	7		7	1	7
39	12	1,5,7,9,11,13	6	1	6	1	6	1		1	11	1
40	6	4,5,8,10,11,13,15,17	11	4	11	4	11	4,5		4,5	11	4
41	10	1,3,4,5,8,9,14	6	3,14	6	3,14	10	--		--	6	--
42	4	1,5,6,7,8,10	11	1	11	1	11	1		1,5	9	1
43	5	1,6,7,10,11,12,13,16	9	1	9	1	9	1		1	9	1
44	12	1,3,5,6,10,11,13	9	1	9	1	9	1		1,6,13,15	9	1

45	8	1,2,3,4,10,11,12,14	8	1,2	8	1,2	8	--	1,2	5	1,2
46	10	1,2,3,4,5,9	7	1	7	1	7	--	1,3,4	11	1
47	9	1,2,3,4,6,10,12,15	11	15	11	--	11	--	10,12,15	11	--
48	8	1,2,3,4,6,10,12,15	6	1	6	1	6	--	1	11	1
49	5	4,6,7,8	5	--	5	--	5	--	--	2	--
50	14	1,2,3,5,11,12,13	14	2,5,12,13	9	12,13	14	--	1,2,12,13	7	--
51	8	1,6,7,9,10,12	3	1,7	8	--	8	--	1,7	3	--
52	11	1,3,5,7,9,12	11	1,7	11	--	11	--	1,7,12	11	--
53	7	1,4,5,6,10	8	1,10	8	10	8	1,10	1,10	7	10
54	5	1,2,3,6,7,11,12	4	1,11	4	1	2	--	1,11	2	1
55	5	2,3,6,7,11,12	5	3	5	--	5	--	3,12	5	--
56	12	1,2,3,6,8,10,11	12	1,2,11	12	11	12	--	11	12	11
57	10	1,2,4,6,7,9,13	14	1,6	14	1	14	1	1	4	1
58	6	2,5,7,8,9,12,13	4	7	4	7	3	5,7	7	3	7
59	12	1,6,7,8,9,13,14	12	1,7	12	1	12	--	1	3	1
60	7	1,2,6,9,11	4	1	4	1	4	--	1,6	10	1
61	7	1,4,8,9,10,12	7	8	7	--	7	--	1,8,9	6	--
62	8	1,2,4,6,10,11,14	9	2,6,14	9	6	9	--	1,2,6,14	9	6
63	7	1,3,8,9,12,13	5	13	5	13	5	--	13	5	13
64	4	1,3,9,10,11,13	6	1,13	6	1,13	4	--	1,13	4	1
65	14	1,2,3,5,8,9,13	12	2,8	12	2,8	12	--	2,8	4	2
66	3	1,6,7,8,11,13	10	1	10	1	10	1,6	1,7,11	3	1
67	11	1,4,6,11,12,13	2	1	2	1	2	1	1	3	1
68	10	1,2,3,4,6,13	9	13	9	13	10	--	1,5,13	7	13
69	10	1,3,4,6,9,13	5	3,13	5	--	5	--	13	10	--
70	12	1,2,6,7,8,11	10	2	12	--	12	--	2	3	--
71	6	1,2,7,9,10,12	11	2,9	11	9	11	9	2,9	11	9
72	2	1,4,5,8,11	2	4,8	2	4,8	2	4	4,8	9	--
73	16	1,2,3,6,9,10,11,12,17	16	1,2	16	1	16	--	1,12	13	1
74	3	1,7,8,10,11,12	9	7	9	7	8	2,4,7	2,3,4,7	5	7
75	8	13,15,16,17,18,19,20,21,22,23,24,25	8	13	8	13	8	--	13,22,23,24,25	18	13
76	8	2,4,6,9,10,12	11	6,9,12	8	9,12	11	4	--	5	--
77	11	1,2,4,5,7,8,12	13	2,8	13	8	13	7,8	1,2,7,8	13	8
78	8	1,2,7,9,10	6	1	6	1	6	1	1	4	1
79	3	1,2,6,10,11,13	3	--	3	--	3	--	--	9	--
80	3	2,7,8,9,12,13,14	10	7,13	10	13	10	--	7,13	3	13
81	7	1,2,6,8,10,12,14,16	15	2	15	2	15	2	1,2,8,10	13	2
82	5	1,2,3,4,9,12,14,17	7	1,12,17	7	1,17	5	17	1,12,17	16	1,17
83	6	1,2,9,11,12,13,14	8	1	8	1	10	--	1,13	8	1
84	5	2,8,10,11,12,13	1	2,8,11	5	--	5	--	2,8	4	--
85	8	1,4,7,10,11,12,13	13	1	13	1	13	1	1,4	2	1
86	17	1,2,3,5,6,8,9,12,15	13	1	13	1	13	1	1,2,6	16	1
87	6	1,2,7,8,10,12,14	6	1,7,8,10,14	6	1,10,14	6	10	1,7,8,10,14	3	10
88	9	1,2,4,5,7,11,14	12	1,2	9	--	9	--	1,2,14	9	--
89	9	1,2,3,10,11,13	7	1	7	--	7	--	1	4	1
90	3	2,5,6,8,9,11,13	3	2,11	10	2	10	2,5	2	7	2
91	7	1,2,5,9,10,13,14,17,18	7	10,18	6	18	7	--	18	4	10,18
92	9	1,2,3,5,7,11	10	1,5	4	5	4	5	1,3,5	10	5
93	7	1,3,4,8,9,11	7	8,9,11	7	--	7	--	--	7	--
94	8	1,2,3,4,6,13	8	1,2,4	7	1	10	--	1,2,4,13	10	1

Table A.2. Spectra FD.

	Data depth theory								PCA			
	DDT_ED_1		DDT_ED_2		DDT_ED_3		DDT_DDT		PCA_Expert		PCA_2	
	30 (100 %)		12 (40 %)		6 (20 %)		0 (0 %)		6 (20 %)		0 (0 %)	
Sample number	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outliers(s)	MRS	Outlier(s)
1	2	1,3	2	1	2	--	2	--		--	4	--
2	4	1,5	4	--	4	--	4	--		--	5	--
3	2	1,3	2	1	2	1	5	--		1	5	--
4	1	2,4	1	4	4	--	1	--		--	3	--
5	5	1,2	5	2	5	2	5	--		--	1	--
6	4	1,2	4	2	3	--	3	--		--	4	--
7	5	1,3	4	--	4	--	4	--		--	5	--
8	4	1,2	5	1	5	1	5	--		1	4	--
9	5	1,4	5	1,4	1	--	1	--		--	3	--
10	1	3,4	5	--	5	--	5	--		--	2	--
11	2	1,4	2	--	2	--	2	--		--	5	--
12	3	2,5	3	--	3	--	3	--		--	2	--
13	4	3,5	1	--	1	--	1	--		--	1	--
14	4	3,5	4	5	4	5	5	--		5	2	--
15	1	3,4	1	--	1	--	1	--		--	4	--
16	5	1,3	5	1	3	--	3	--		--	3	--
17	2	1,5	4	--	4	--	4	--		--	3	--
18	2	1,3	2	1	2	--	2	--		--	5	--
19	5	1,2	5	--	5	--	5	--		1	5	--
20	5	2,4	2	--	2	--	2	--		--	4	--
21	4	2,5	4	--	4	--	4	--		--	5	--
22	3	1,2	3	--	3	--	3	--		--	5	--
23	4	1,5	4	1	4	1	5	--		1	3	--
24	5	1,4	4	1	4	1	5	--		1	2	--
25	1	3,5	3	--	3	--	3	--		--	4	--
26	4	3,5	4	--	4	--	4	--		--	4	--
27	3	1,2	4	--	4	--	4	--		--	3	--
28	4	2,3	2	--	2	--	2	--		--	3	--
29	1	2,3	5	--	5	--	5	--		--	5	--
30	1	2,4	2	--	2	--	2	--		--	3	--

Table A.3. Spectra FU.

	Data depth theory								PCA			
	DDT_ED_1		DDT_ED_2		DDT_ED_3		DDT_DDT		PCA_Expert		PCA_2	
	30 (100 %)		7 (23 %)		4 (13 %)		0 (0 %)		6 (20 %)		0 (0 %)	
Sample number	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outliers(s)	MRS	Outlier(s)
1	2	1,4	2	1	2	1	5	--		1	4	--
2	3	2,5	1	--	1	--	1	--		--	5	--
3	2	1,4	4	--	4	--	4	--		--	4	--
4	2	3,5	2	--	2	--	2	--		--	5	--
5	5	2,3	5	--	5	--	5	--		--	5	--
6	1	4,5	1	--	1	--	1	--		--	5	--
7	2	1,5	2	--	2	--	2	--		--	1	--
8	4	2,3	3	--	3	--	3	--		--	4	--
9	3	1,2	2	1	2	1	5	--		1	2	--
10	2	1,3	2	--	2	--	2	--		1	2	--
11	1	2,5	5	--	5	--	5	--		--	5	--
12	1	3,5	1	--	1	--	1	--		--	4	--
13	3	2,5	3	--	3	--	3	--		--	3	--
14	4	2,3	4	--	4	--	4	--		--	5	--
15	2	3,4	3	--	3	--	3	--		--	5	--
16	3	1,2	2	--	2	--	2	--		--	3	--
17	3	1,4	4	--	4	--	4	--		--	2	--
18	4	1,2	4	1	4	--	4	--		--	2	--
19	2	1,4	2	4	2	--	2	--		--	3	--
20	2	1,4	5	--	5	--	5	--		--	2	--
21	3	1,4	3	1	3	--	3	--		1	4	--
22	1	2,3	5	--	5	--	5	--		--	5	--
23	4	1,2	3	--	3	--	3	--		--	4	--
24	2	1,3	3	1	3	1	5	--		1	4	--
25	1	2,4	4	--	4	--	4	--		--	2	--
26	2	3,5	2	--	2	--	2	--		--	2	--
27	1	2,4	1	--	1	--	1	--		--	5	--
28	5	2,4	5	--	5	--	5	--		--	3	--
29	4	1,2	1	--	1	--	1	--		--	4	--
30	5	1,3	3	1	3	1	5	--		1	2	--

Table A.4. Spectra UD.

	Data depth theory								PCA			
	DDT_ED_1		DDT_ED_2		DDT_ED_3		DDT_DDT		PCA_Expert		PCA_2	
	30 (100 %)		4 (13 %)		3 (10 %)		0 (0 %)		2 (7 %)			
Sample number	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outliers(s)	MRS	Outlier(s)
1	2	1,5	5	1	5	1	5	--		--	5	--
2	4	2,3	4	--	4	--	4	--		--	3	--
3	2	1,4	2	--	2	--	2	--		--	3	--
4	3	1,2	3	2	4	--	4	--		--	5	--
5	5	2,4	4	--	4	--	4	--		1	5	--
6	1	3,4	3	--	3	--	3	--		--	1	--
7	2	1,5	5	--	5	--	5	--		--	2	--
8	4	2,3	4	--	4	--	4	--		--	1	--
9	5	1,4	5	1	5	1	5	--		--	2	--
10	4	2,3	2	--	2	--	2	--		--	3	--
11	1	2,5	2	--	2	--	2	--		--	3	--
12	4	3,5	5	--	5	--	5	--		--	4	--
13	2	4,5	5	--	5	--	5	--		--	2	--
14	2	4,5	3	--	3	--	3	--		--	2	--
15	2	3,4	3	--	3	--	3	--		--	3	--
16	5	1,3	3	--	3	--	3	--		--	5	--
17	4	1,5	4	--	4	--	4	--		--	3	--
18	4	2,3	4	--	4	--	4	--		--	4	--
19	2	1,5	2	1	2	1	5	--		--	2	--
20	3	1,5	3	--	3	--	3	--		--	4	--
21	3	1,5	3	--	3	--	3	--		1	4	--
22	5	1,3	5	--	5	--	5	--		--	3	--
23	3	1,2	3	--	3	--	3	--		--	5	--
24	2	3,4	2	--	2	--	2	--		--	5	--
25	3	4,5	3	--	3	--	3	--		--	4	--
26	2	3,5	4	--	4	--	4	--		--	5	--
27	4	3,5	4	--	4	--	4	--		--	1	--
28	2	3,4	3	--	3	--	3	--		--	2	--
29	3	2,5	4	--	4	--	4	--		--	3	--
30	1	4,5	4	--	4	--	4	--		--	5	--

Table A.5. Spectra UU.

	Data depth theory								PCA			
	DDT_ED_1		DDT_ED_2		DDT_ED_3		DDT_DDT		PCA_Expert		PCA_2	
	30 (100 %)		4 (13 %)		1 (3 %)		0 (0 %)		5 (17 %)			
Sample number	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outlier(s)	MRS	Outliers(s)	MRS	Outlier(s)
1	2	1,3	5	--	5	--	5	--		1	5	--
2	4	1,2	4	--	4	--	4	--		--	4	--
3	2	1,4	2	--	2	--	2	--		--	2	--
4	3	2,4	3	--	3	--	3	--		--	4	--
5	5	1,2	5	1	5	1	5	--		--	3	--
6	4	1,2	1	--	1	--	1	--		--	3	--
7	1	3,5	1	--	1	--	1	--		--	1	--
8	2	3,5	2	--	2	--	2	--		1	5	--
9	1	3,5	1	--	1	--	1	--		--	5	--
10	4	1,2	5	--	5	--	5	--		1,2,3,4,5	1	--
11	3	1,2	3	2	3	--	3	--		--	5	--
12	5	1,4	5	--	5	--	5	--		--	5	--
13	1	2,4	1	--	1	--	1	--		--	5	--
14	1	3,4	1	--	1	--	1	--		--	3	--
15	4	1,5	1	--	1	--	1	--		--	5	--
16	2	1,5	2	--	2	--	2	--		--	3	--
17	2	1,3	2	1,3	2	--	2	--		--	4	--
18	4	2,5	4	--	4	--	4	--		--	2	--
19	4	1,3	5	--	5	--	5	--		1	3	--
20	3	1,4	3	--	3	--	3	--		--	3	--
21	2	1,5	5	--	5	--	5	--		1	3	--
22	5	2,4	5	--	5	--	5	--		--	3	--
23	4	1,2	4	--	4	--	4	--		--	3	--
24	5	3,4	5	--	5	--	5	--		--	2	--
25	3	2,4	5	4	3	--	3	--		--	3	--
26	2	4,5	4	--	4	--	4	--		--	4	--
27	1	4,5	1	--	1	--	1	--		--	2	--
28	1	3,4	4	--	4	--	4	--		--	5	--
29	3	2,5	3	--	3	--	3	--		--	4	--
30	4	3,5	2	--	2	--	2	--		--	5	--

Appendix B: Detailed results

Table B.1. Summary of outlier detection by the different methods for each data set (sub table). Each method (row) is compared to a reference method (column) according to the following statistics: TP-TN/FP-FN. The numbers of samples identified as containing outliers are below the method names.

	WWTP (94 samples)					
Method	DDT_ED_194	DDT_ED_289	DDT_ED_369	DDT_DDT39	PCA_Expert82	PCA_260
DDT_ED_1	-	89 - 0 / 5 - 0	69 - 0 / 25 - 0	39 - 0 / 55 - 0	82 - 0 / 12 - 0	60 - 0 / 34 - 0
DDT_ED_2		-	69 - 5 / 20 - 0	41 - 5 / 48 - 0	81 - 3 / 9 - 1	60 - 6 / 28 - 0
DDT_ED_3			-	39 - 25 / 29 - 1	66 - 8 / 4 - 16	60 - 22 / 10 - 2
DDT_DDT				-	38 - 11 / 1 - 44	34 - 29 / 5 - 26
PCA_Expert					-	58 - 11 / 23 - 2
PCA_2						-

	FD (30 samples)					
Method	DDT_ED_130	DDT_ED_212	DDT_ED_36	DDT_DDT0	PCA_Expert6	PCA_20
DDT_ED_1	-	12 - 0 / 18 - 0	6 - 0 / 24 - 0	0 - 0 / 30 -0	6 - 0 / 24 - 0	0 - 24 / 6 - 0
DDT_ED_2		-	6 - 18 / 6 - 0	0 - 18 / 12 - 0	5 - 17 / 7 - 1	0 - 30 / 0 - 0
DDT_ED_3			-	0 - 24 / 6 - 0	5 - 23 / 2 -1	0 - 24 / 6 - 0
DDT_DDT				-	0 - 24 / 0 - 6	0 - 18 / 12 - 0
PCA_Expert					-	0 - 0 / 30 - 0
PCA_2						-

	FU (30 samples)					
Method	DDT_ED_130	DDT_ED_27	DDT_ED_34	DDT_DDT0	PCA_Expert6	PCA_20
DDT_ED_1	-	7 - 0 / 23 - 0	4 - 0 / 26 - 0	0 - 0 / 30 - 0	6 - 0 / 24 - 0	0 - 0 / 30 - 0
DDT_ED_2		-	4 - 23 / 3 - 0	0 - 23 / 7 - 0	5 - 22 / 2 - 1	0 - 23 / 7 - 0
DDT_ED_3			-	0 - 26 / 4 - 0	4 - 24 / 0 - 2	0 - 26 / 4 - 0
DDT_DDT				-	0 - 24 / 0 - 6	0 - 30 / 0 - 0
PCA_Expert					-	0 - 24 / 6 - 0
PCA_2						-

	UD (30 samples)					
Method	DDT_ED_130	DDT_ED_24	DDT_ED_33	DDT_DDT0	PCA_Expert2	PCA_20
DDT_ED_1	-	4 - 0 / 26 - 0	3 - 0 / 27 - 0	0 - 0 / 30 - 0	2 - 0 / 28 - 0	0 - 0 / 30 - 0
DDT_ED_2		-	3 - 26 / 1 - 0	0 - 26 / 4 - 0	0 - 24 / 4 - 2	0 - 26 / 4 - 0
DDT_ED_3			-	0 - 27 / 3 - 0	0 - 25 / 3 - 2	0 - 27 / 3 - 0
DDT_DDT				-	0 - 28 / 0 - 2	0 - 30 / 0 - 0
PCA_Expert					-	0 - 28 / 2 - 0
PCA_2						-

	UU (30 samples)					
Method	DDT_ED_130	DDT_ED_24	DDT_ED_31	DDT_DDT0	PCA_Expert5	PCA_20
DDT_ED_1	-	4 - 0 / 26 - 0	1 - 0 / 29 - 0	0 - 0 / 30 - 0	5 - 0 / 25 - 0	0 - 0 / 30 - 0
DDT_ED_2		-	1 - 26 / 3 - 0	0 - 26 / 4 - 0	0 - 21 / 4 - 5	0 - 26 / 4 - 0
DDT_ED_3			-	0 - 29 / 1 - 0	0 - 24 / 1 - 5	0 - 29 / 1 - 0
DDT_DDT				-	0 - 25 / 0 - 5	0 - 30 / 0 - 0
PCA_Expert					-	0 - 25 / 5 - 0
PCA_2						-

Table B.2. Summary of outlier identification by the different methods for each data set (sub table). Each method (row) is compared to a reference method (column) according to the consistency ratios in outlier identification. The numbers of samples containing outliers are below the method names. NSWOIC = No Sample With Outlier In Common.

	WWTP (94 samples)					
Method	DDT_ED_194	DDT_ED_289	DDT_ED_369	DDT_DDT39	PCA_Expert82	PCA_260
DDT_ED_1	1	1	1	1	0.99	1
DDT_ED_2		1	1	1	1	1
DDT_ED_3			1	0.97	0.99	0.99
DDT_DDT				1	0.98	0.99
PCA_Expert					1	1
PCA_2						1

	FD (30 samples)					
Method	DDT_ED_130	DDT_ED_212	DDT_ED_36	DDT_DDT0	PCA_Expert6	PCA_20
DDT_ED_1	1	1	1	--	1	--
DDT_ED_2		1	1	--	1	--
DDT_ED_3			1	--	1	--
DDT_DDT				1	--	--
PCA_Expert					1	--
PCA_2						1

	FU (30 samples)					
Method	DDT_ED_130	DDT_ED_27	DDT_ED_34	DDT_DDT0	PCA_Expert6	PCA_20
DDT_ED_1	1	1	1	--	1	--
DDT_ED_2		1	1	--	1	--
DDT_ED_3			1	--	1	--
DDT_DDT				1	--	--
PCA_Expert					1	--
PCA_2						1

	UD (30 samples)					
Method	DDT_ED_130	DDT_ED_24	DDT_ED_33	DDT_DDT0	PCA_Expert2	PCA_20
DDT_ED_1	1	1	1	--	0.5	--
DDT_ED_2		1	1	--	NSWOIC	--
DDT_ED_3			1	--	NSWOIC	--
DDT_DDT				1	--	--
PCA_Expert					1	--
PCA_2						1

	UU (30 samples)					
Method	DDT_ED_130	DDT_ED_24	DDT_ED_31	DDT_DDT0	PCA_Expert5	PCA_20
DDT_ED_1	1	1	1	--	1	--
DDT_ED_2		1	1	--	NSWOIC	--
DDT_ED_3			1	--	NSWOIC	--
DDT_DDT				--	--	--
PCA_Expert					1	--
PCA_2						--

Table B.3. Summary of MRS identification by the different methods for each data set (sub table). Each method (row) is compared to a reference method (column) according to the following statistics: consistency ratios for the identification of the MRS: from 0 (never the same) to 1 (always the same).

	WWTP (94 samples)				
Method	DDT_ED_1	DDT_ED_2	DDT_ED_3	DDT_DDT	PCA_2
DDT_ED_1	1	0.35	0.35	0.41	0.11
DDT_ED_2		1	0.81	0.71	0.13
DDT_ED_3			1	0.87	0.24
DDT_DDT				1	0.3
PCA_2					1

	FD (30 samples)				
Method	DDT_ED_1	DDT_ED_2	DDT_ED_3	DDT_DDT	PCA_2
DDT_ED_1	1	0.6	0.47	0.43	0.2
DDT_ED_2		1	0.87	0.77	0.17
DDT_ED_3			1	0.83	0.17
DDT_DDT				1	0.2
PCA_2					1

	FU (30 samples)				
Method	DDT_ED_1	DDT_ED_2	DDT_ED_3	DDT_DDT	PCA_2
DDT_ED_1	1	0.5	0.5	0.5	0.3
DDT_ED_2		1	1	0.87	0.27
DDT_ED_3			1	0.87	0.27
DDT_DDT				1	0.23
PCA_2					1

	UD (30 samples)				
Method	DDT_ED_1	DDT_ED_2	DDT_ED_3	DDT_DDT	PCA_2
DDT_ED_1	1	0.5	0.47	0.43	0.37
DDT_ED_2		1	0.97	0.97	0.13
DDT_ED_3			1	0.97	0.13
DDT_DDT				1	0.1
PCA_2					1

	UU (30 samples)				
Method	DDT_ED_1	DDT_ED_2	DDT_ED_3	DDT_DDT	PCA_2
DDT_ED_1	1	0.67	0.7	0.7	0.2
DDT_ED_2		1	0.97	0.97	0.23
DDT_ED_3			1	1	0.27
DDT_DDT				1	0.27
PCA_2					1