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A NEW APPROACH FOR SPECTRA BASELINE CORRECTION USING SPARSE REPRESENTATION

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ABSTRACT
A new baseline correction algorithm for spectral signal based on sparse representation is proposed. Firstly, utilizing the training sample to obtain the dictionaries of both baseline and spectrum; Secondly, establishing sparse representation model of spectral signal; thirdly, employing OMP algorithm to calculate the representation coefficients of spectral signal and finally, obtaining the spectral baseline from representation coefficients which are corresponded to the baseline dictionary. Then, the spectra baseline correction is completed by removing the baseline from original observed spectrum. Contrast experiment and quantitative analysis of corrected spectral signals are conducted and results show the highly efficiency and accuracy of the proposed algorithm.

KEY WORDS
Spectral baseline correction; Sparse; Dictionary learning; KSVD algorithm; OMP; Quantitative analysis

1 Introduction

Fourier transform infrared spectroscopy(FTIR) is a useful method for both qualitative and quantitative analysis in Analytic Chemistry. However, due to ageing of device as well as different influence factors for spectra collection, like temperature, pressure and humidity, baseline drift can often be observed in different signals. These drifted baselines seriously influence the interpretation of spectra as well as the accuracy and robustness of the quantitative analysis model. Therefore, it is necessary to remove the baseline drift in spectroscopic analysis.

Baseline correction is to pull the drifted baseline to zero absorption location and it must be taken into consideration in many fields[1]:Infrared spectroscopy[2, 3], Nuclear Magnetic Resonance[4, 28], Raman spectroscopy[6],Chromatography[7], X-ray[8],γ-ray[9] and Electrocardiography[10, 11].

Usually,the baseline can be regarded as a background which changes slowly[12]. However, there is no mathematical definition to it at present. According to different assumptions, many approaches are proposed: (1)derivative method; (2)frequency or time-frequency domain; (3)local mid-value; (4) curve fitting; (5)background estimation; (6)morphology filter; (7)asymmetric least squares; (8)robust local regression.

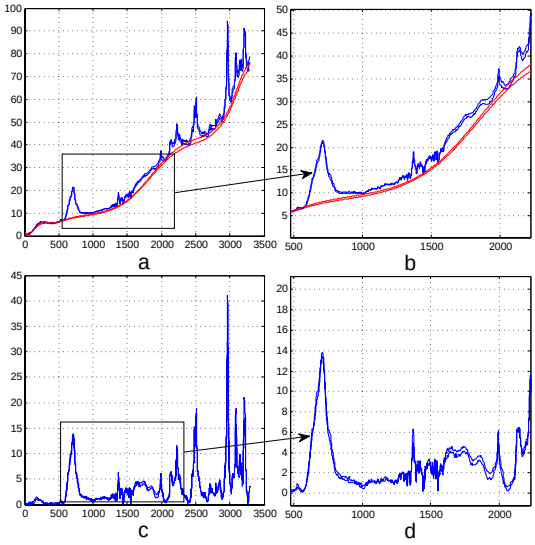

Figure 1. Result of proposed algorithm: (a) is the original spectral signal (blue) and the obtained baseline(red) with our proposed algorithm, (c) is the spectral signal with baseline correction, (b) and (d) are zoomed in details of (a) and (c), respectively.

Derivative method is a common used approach in baseline correction. Commonly, first order derivative can remove the constant component and second order derivative can be used to remove the constant and linear components. But, derivative operation will amplify noises, which means the signal after derivation should be processed via filter. Usually, an appropriate band pass filter is employed to instantaneously suppress the baseline and noise. But this method can not thoroughly remove the baseline.

Converting the spectral signal into frequency or time-frequency domain is the so-called frequency or time-frequency based method. Fourier transform and wavelet transform are two widely used transforms. We can eliminate the drifted baseline according to the frequency differ-

ence character between baseline and signal which is based on the fundamental assumption that baseline is the low frequency of observed spectrum. However, the choice of filter parameters is challenging and fourier transform is highly sensitive to noises. By employing wavelet transform, spectrum can be decomposed into detail and approximation signal. Approximation component represents the low frequency of spectrum which can be regarded as the approximation of the baseline. But the wavelet-based baseline correction usually pulls the spectrum below zero. It disobeys with the actual situation.

Curve fitting algorithm can calculate drifting baseline from original spectrogram via fitting. The key of the method depends on the finding of the interpolation nodes which can represent features of the baseline. In addition, we commonly choose nodes based on partial minimum points of signal. However, threshold normally is determined by human experience which relates to the signal and has a significant effect over the method. Gan and Lieber [13]have put forward a method based on the iteration of polynomial which can automatically determine the threshold. But we must set the order of polynomial and in which way the iteration will be terminated (the maximum iteration time or the convergent threshold) in advance.

In 2004, Eilers proposed AsLS baseline correction algorithm which is based on Whittaker smoothing to minimize cost function[27]:

$$Q = \sum_i w_i (y_i - z_i)^2 + \mu \sum_i (\Delta^2 z_i)^2 \qquad (1)$$

y is the given spectrogram, and z is a smoothing approximation of y, Δ is the difference operator, w is the asymmetric weight. Positive μ is a regularization parameter which determines the degree of smoothness punishment. The baseline is smoother when μ is bigger. The estimation of the baseline represents the elimination of peaks, and the weights are chosen to refuse the influence of peaks.However, the accuracy of parameters commonly depend on judgment of human which needs strong professional background.

In fact, Ryan, Morhac, Ruckstuhl and many other researchers all have proposed different methods for baseline correction, and all of these methods have their own limitations or drawbacks in different situations. Therefore, in this paper, we proposed a new algorithm for baseline correction and our new algorithm can be used in different situations and can also keep high accuracy in different situations.

The remainder of this paper is organized as follows: In section(2), fundamental of FTIR is briefly introduced and a new algorithm for baseline correction based on sparse model is presented in section(3). Then, in section(4), experiment results and results analysis are presented, and finally, in section(5), the conclusions are drawn.

2 Lambert-Beer's Law

The theoretical fundamental of quantitative analysis using infrared spectrum is Lambert-Beer's Law. When a bundle of parallel monochromatic light is radiating on the solution, part of the light is absorbed by the solution (which we call the absorption light I_a),the second part of the light transmits through the solution (which we call the transmission light I),the final part is reflected as the reflection light I_r.If the incident light is I_o,then $I_o = I_a + I + I_r$.Usually, the reflective rate of container is constant, in addition, it can also decrease to a minimum value, thus $I_o \simeq I_a + I$.

Lambert's Law:when a bunch of monochromatic light with certain wavelength transmits through a homogeneous solution of certain concentration, the absorption intensity of light is proportional to the thickness of the liquid layer b and the incident light intensity[15]:

$$\lg \frac{I_0}{I} = a_1 b \qquad (2)$$

Beer's Law: when a bunch of a monochromatic light with certain wavelength transmits through solution with the constant thickness of the solution layer and homogeneous absorption of light, then the solution concentration will increase dC, and the intensity of light will be weakened by $-dI$, in addition, $-dI$ is proportional to the transmitted light intensity I and dC.

$$\lg \frac{I_0}{I} = a_2 c \qquad (3)$$

When the above two laws are combined into a single one, that is Lambert-Beer Law, and is referred to as Beer's law.

$$\lg \frac{I_0}{I} = abc \qquad (4)$$

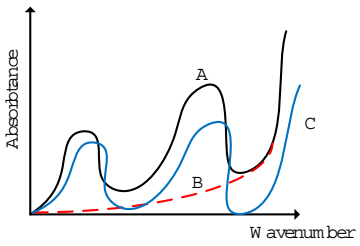

Figure 2. The meaning of baseline correction: A is the original spectral signal with drifted baseline which contradicts with linear relationship in Bill Lambert's law, B is the drifted baseline, C is the corrected spectral signal which meets Bill Lambert's law.

Strictly speaking, Beer's law can only be applied to monochromatic light, however, the slit of dispersive infrared spectrometer has a certain width , which means the obtained monochromatic light also contains a narrow range of polychromatic lights with different wave numbers. In addition, the wider of the slit, the greater error of Beer's

law. But if slit width is too small, the Signal-Noise Ratio(SNR) will be decreased. Therefore, the smaller width of slit is better with a specific SNR.

Another factor of dispersive instrument that can influence Beer's law is the presence of stray light which can make absorption peaks move to the direction of higher wave number and the absorption strength be weakened, thereby affecting the linear relationship in Bill Lambert law and causing the drift of baseline in spectral signal(Fig.2).

3 New Approach for Baseline Correction Using Sparse Model

3.1 Model Overview

The overall flow is shown as Fig(3). Assume that we have a set of samples which can be divided into two separately parts, one is the corrected spectral signals, and the other is consisted of signals without baseline correction. Let y, b, s,ε be the observed spectral signal, baseline, source spectrum and energy limited additive component respectively. Commonly, we can model them using:

$$y = s + b + \varepsilon \tag{5}$$

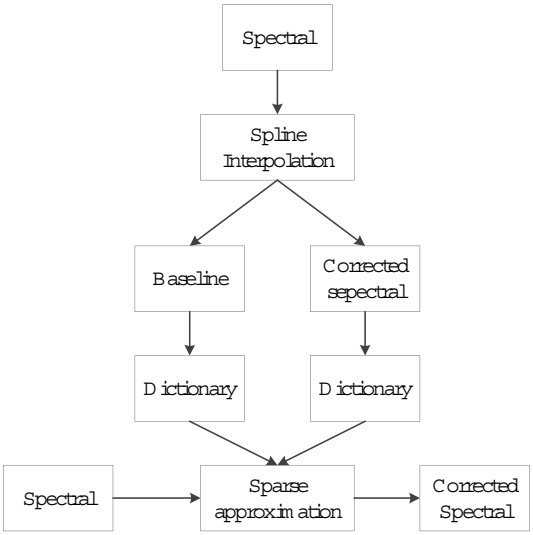

Figure 3. Flow

Our goal is to learn from these sample in order to approximate the signal via simple and computationally efficient scheme. Given sufficient training samples of ith class,where $i = 1, 2$ represents the source spectrum and the baseline respectively. In learning procedure, we begin with a set of samples, which is consisted of baseline and source spectrum, as Fig(4). Consider a set of source spectra $\mathbf{S} = \{\mathbf{s}_i\}_{i=1}^{N}, s \in \mathbf{R}^n$. Our aim is to learn a dictionary $D_s \in \mathbf{R}^{n\times m}$ over which $\mathbf{Y}$ has a sparse representation $\boldsymbol{\alpha}_s$. This can be written as an optimization problem[16]:

$$\min_{\boldsymbol{D}_s,\boldsymbol{\alpha}_s} \|\boldsymbol{Y} - \boldsymbol{D}_s\boldsymbol{\alpha}_s\|_F^2 \text{s.t} \|\alpha\|_0 \le t \tag{6}$$

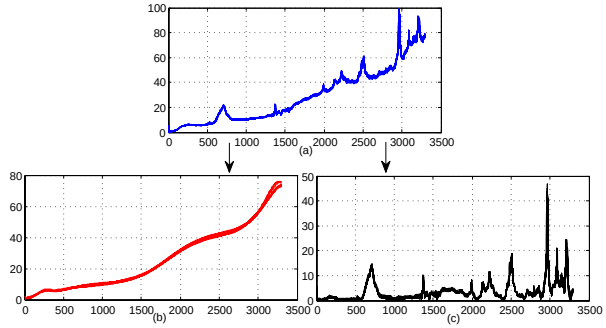

Figure 4. Training sample:Training sample: (b) is baseline and (c) is source spectrum.

To obtain a baseline from a observed spectrum, we use a sparse model to approximate the observed signal

$$\arg\min_{\boldsymbol{\alpha}_s,\boldsymbol{\alpha}_b} \|\boldsymbol{\alpha}_s\|_0 + \|\boldsymbol{\alpha}_b\|_0, \text{s.t.} \|\boldsymbol{Y} - \boldsymbol{D}_s\boldsymbol{\alpha}_s - \boldsymbol{D}_b\boldsymbol{\alpha}_b\|_2^2 \le \varepsilon \tag{7}$$

where $\|\cdot\|_0$ is the ℓ^0-norm that counts the number of nonzero entries which is known as a NP-hard problem[19]. We can equivalently solve (8) via $\|\cdot\|_1$

$$\arg\min_{\boldsymbol{\alpha}_s,\boldsymbol{\alpha}_b} \|\boldsymbol{\alpha}_s\|_1 + \|\boldsymbol{\alpha}_b\|_1, \text{s.t.} \|\boldsymbol{Y} - \boldsymbol{D}_s\boldsymbol{\alpha}_s - \boldsymbol{D}_b\boldsymbol{\alpha}_b\|_2^2 \le \varepsilon \tag{8}$$

Bruckstein[17]pointed out that there are appropriate γ_s, γ_b to make (8) be equivalent to[20, 21, 22, 23]:

$$\arg\min_{\boldsymbol{\alpha}_s,\boldsymbol{\alpha}_b} \|\boldsymbol{Y} - \boldsymbol{D}_s\boldsymbol{\alpha}_s - \boldsymbol{D}_b\boldsymbol{\alpha}_b\|_2^2 + \gamma_s\|\boldsymbol{\alpha}_s\|_1 + \gamma_b\|\boldsymbol{\alpha}_b\|_1 \tag{9}$$

Let $\gamma = \gamma_1 = \gamma_2$,$\boldsymbol{D} = [\boldsymbol{D}_s\boldsymbol{D}_b]$,$\boldsymbol{\alpha} = [\boldsymbol{\alpha}_s\boldsymbol{\alpha}_b]^T$,(9) can be rewritten as:

$$\arg\min_{\boldsymbol{\alpha}} \|\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{\alpha}\|_2^2 + \gamma\|\boldsymbol{\alpha}\|_1 \tag{10}$$

According to (10) and practical application, we should take three aspects into consideration.

3.2 Dictionary Learning

The next procedure is to learn the dictionaries and the corresponding sparse representation coefficients. To begin with, we briefly describe the dictionary learning algorithm.

Consider a set of samples $\boldsymbol{Y} = \{\boldsymbol{y}_i\}_{i=1}^{p}, \boldsymbol{y}_i \in \mathbf{R}^n$. We wish to learn a dictionary $\boldsymbol{D} \in \mathbf{R}$ over which $\boldsymbol{Y}$ has a sparse representation $\boldsymbol{\alpha} = \{\alpha\}_{i=1}^{p}, \alpha \in \mathbf{R}^m$ such that each α_i contains $k(k \ll n)$ nonzero elements. This is formally written as:

$$\min_{\Phi,\boldsymbol{X}} \|\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{\alpha}\|_F^2 \text{ subject to } \|\boldsymbol{\alpha}\|_0 \le k \tag{11}$$

where the $\|\cdot\|_F$ is the Frobenius norm and $\|\cdot\|_0$ is the ℓ_0 norm. Solving (11),a newly developed dictionary learning algorithm K-SVD is used. K-SVD iteratively solves (11)

by performing two steps at every iteration: (1)sparse coding and(2)dictionary update. And in the sparse coding step, $\boldsymbol{D}$ is fixed and $\boldsymbol{\alpha}$ is computed.

$$\min_{\boldsymbol{X}} \|\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{\alpha}\|_F^2 \text{ subject to } \|\boldsymbol{\alpha}\|_0 \leq k \qquad (12)$$

In (12) there is ℓ_0 term which makes the problem to be a NP-hard. Some approaches such as Matching Pursuit(MP), Orthogonal Matching Pursuit(OMP) are employed for solving (12), BP replace the ℓ_0 norm with ℓ_1 penalty in order to convert the problem into a convex one. In the original K-SVD, the OMP is utilized because it is fast, easy to implement and of fairly accuracy. For this reason, we use OMP to solve all sparse approximation in this paper.

In dictionary update procedure, the atom of dictionary $\boldsymbol{D}$ are updated sequentially, allowing the relevant coefficients in $\boldsymbol{\alpha}$ to change as well. Updating an atom in $\boldsymbol{D}$ involves computing a rank-one approximation of residual matrix

$$\mathbf{E}_i = \mathbf{Y} - \widetilde{\boldsymbol{D}}_i \widetilde{\boldsymbol{\alpha}}_i \qquad (13)$$

where $\widetilde{\boldsymbol{D}}_i$ and $\widetilde{\boldsymbol{\alpha}}_i$ are formed by removing the ith column from $\boldsymbol{D}$ and ith row from $\boldsymbol{\alpha}$. This rank-one approximation is computed by subjecting $\boldsymbol{E}_i$ to a singular value decomposition(SVD).

In this paper, we have two classes which means we should consider:(1)learning two dictionaries, one for source spectrum and the other for baseline and (2)a single dictionary formed by concatenating two class-specific dictionaries.

3.3 Algorithm for the Model

Once the dictionary is obtained, we can employ reliable and efficient method to solve (10). The Orthogonal Matching Pursuit(OMP) is briefly introduced in Table(1).

Table 1. Orthogonal Matching Pursuit

Orthogonal Matching Pursuit for Approximating the Solution
Aim: Approximate the solution: $\arg\min_{\boldsymbol{\alpha}} \|\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{\alpha}\|_2^2 + \gamma\|\boldsymbol{\alpha}\|_1$
Known data: Dictionary $\boldsymbol{D}$ and the observed infrared spectral $\boldsymbol{Y}$, and error threshold ε_0;
Initialization: (1)Iterative number $k = 0$; (2)Solution: $\boldsymbol{\alpha}^0 = \mathbf{0}$; (3)Residual: $\boldsymbol{r}^0 = \boldsymbol{Y} - \boldsymbol{D}\boldsymbol{\alpha}^0 = \boldsymbol{b}$ (4)Solution support: $\mathbf{S} = support\{\boldsymbol{\alpha}^0\}$
Iterative Procedure: $k \leftarrow k + 1$ and perform the following steps:
(1)**Sweep**: computing the error $\varepsilon(j) = \min_{z_j} = \|\boldsymbol{d}_j z_j - \boldsymbol{r}^{k-1}\|_2^2$ for all j using the optimal $z_j^* = \boldsymbol{d}_j^T \boldsymbol{r}^{k-1}/\|\boldsymbol{d}_j\|_2^2$;
(2)**Update Support**: Search a minimizer, j_0 of $\varepsilon(j) : \forall j \notin \mathbf{S}^{k-1}$, $\varepsilon(j_0) \leq \varepsilon(j)$update $\mathbf{S}^k = \mathbf{S}^{k-1} \bigcup \{j_0\}$
(3)**Update Provisional Solution**: Compute $\boldsymbol{\alpha}^k$, the minimizer of $\|\boldsymbol{D}\boldsymbol{\alpha} - \boldsymbol{Y}\|_2^2$ subject to $support\{\boldsymbol{\alpha}\} = \mathbf{S}^k$
(4)**Update Residual**: Compute $\boldsymbol{r}^k = \boldsymbol{Y} - \boldsymbol{D}\boldsymbol{\alpha}^k$
(5)**Stopping criteria**: If $\|\boldsymbol{r}^k\|_2 < \varepsilon_0$, stop. Else apply another iteration.
Output: Solution $\boldsymbol{\alpha}^k$

4 Experiment

We have conducted two types of experiments using sparse model. In the first type, we use the proposed method for baseline correction and compare with other method and, in the second type, we have conducted experiments to compare the quantitative analysis results using widely used approaches include: Multiple Scattering Correction(MSC), Normalization, First or Second Order Derivative(FOD or SOD), Discrete Wavelet Transform(DWT), EMD[24, 25], Ryan's method[26], AsLS[27], Fiedrich[28] and our proposed algorithm.

4.1 Baseline Correction Using Proposed Method

In this subsection we employ the proposed algorithm, DWT, EMD, Firedrichs's method, Ryan's method and Eilers's method to correct baseline. The aim of experiments in this section is to verify the efficiency of our proposed method. Fig(5) is the data employed for the experiments.

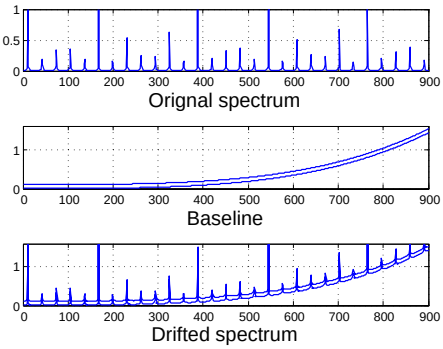

Figure 5. Synthetic data for experiment: (a) is our source spectral signal, (b) is our synthesized baseline, (c) is the drifted spectral signal with our synthesized baseline.

The baseline correction results using our proposed algorithm, DWT, EMD, AsLS, Fiedrich are shown in Fig(6) respectively. When employing DWT,the spectral are decomposed into eight layers with db10 wavelet, and the lowest frequency component is baseline. When employing EMD, the spectral are decomposed into ten layers, and the lowest frequency component is baseline. The weight $p = 0.001$, and the regularization parameter $\lambda = 10^8$ when employing AsLS. The window size $W = 23$ when using Fiedrich's method.

As is shown in the figure, our proposed algorithm can effectively and efficiently detect the baseline as well as correct the spectrum signal compared with other algorithms.

4.2 Quantitative Analysis Comparison

In this section we give the result of quantitative analysis with our proposed approach and other frequently used methods. We collect the infrared spectra with Thermo

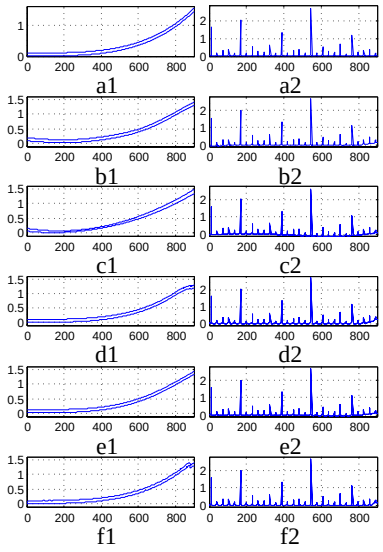

Figure 6. Baseline correction with different algorithms: (a1),(b1),(c1),(d1),(e1),(f1) are detected baseline with our proposed algorithm, DWT, EMD, Ryan, AsLS and Fiedrich, respectively; (a1),(b2),(c2),(d2),(e2),(f2) are corrected spectral signals corresponding to each algorithms.

Table 2. Samples for quantitative analysis

NO	Ethanol	Ethyl acetate	Ethanol+ethyl acetate
1	0.00%	0.50g/L	1.14g/L
2	2.00%	1.00g/L	1.25g/L
3	5.26%	1.40g/L	1.40g/L
4	11.1%	1.60g/L	1.60g/L
5	25.00%	1.80g/L	1.80g/L
6	30.00%	2.00g/L	-
7	40.00%	2.20g/L	-
8	50.00%	2.50g/L	-

Nicolet infrared spectrometry. The samples are the ethanol solution with different volume ratio, ethyl acetate aqueous solution with different concentration, as well as aqueous solution of ethyl acetate and ethanol with different concentration. Specific information is shown in Table(4.2). In analytical chemistry, Partial Least Squares(PLS) is a wildly used method for quantitative analysis. In our experiments, we utilized five spectral as the training samples and the remaining three as the testing samples to build a PLS based model for ethanol concentration quantitative analysis. The results are shown in Fig(7) and Fig(9).

From the experimental results, we can demonstrate that our algorithm is always with the minimum error when be applied in quantitative analysis.

5 Conclusion

In this paper, we have proposed a new algorithm for baseline correction in spectral signal with sparse representation. Our proposed algorithm can be utilized in different situations when related to baseline correction for one dimensional signal and is with highly efficiency as well as accuracy compared with other traditional methods.

In our experiments, the validating performance of our proposed algorithm is presented. As is shown, our algorithm can effectively extract the baseline of spectrum and can accurately remove the baseline of spectrum compared with many other conventional methods. In addition, our algorithm always keeps the minimum error when be applied in quantitative analysis in analytical chemistry.

In the future, the algorithm described in this paper could be improved and extended works would be done in the following areas. Firstly, a new baseline correction algorithm based on blind source separation will be proposed which is more effective than any other conventional algorithms, and secondly, another algorithm with Manhattan non-negative matrix factorization will be proposed, and the related work has begun.

6 Acknowledgements

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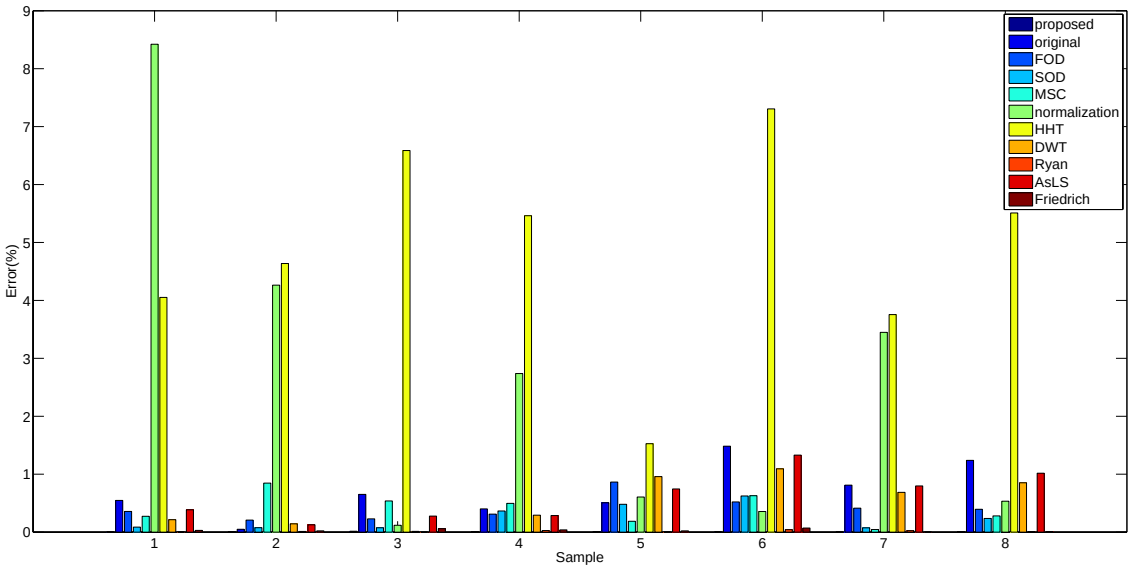

Figure 7. Result of contrast experiment: Analytical errors are displayed as bar graphs.

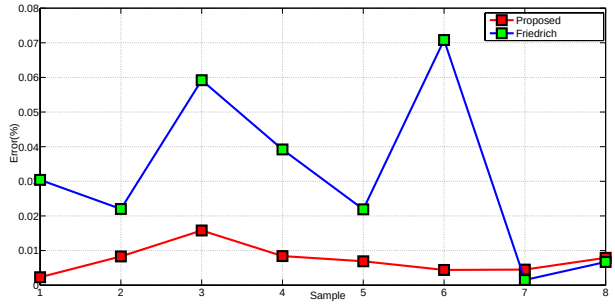

Figure 8. Details of comparative information between our proposed algorithm and Friedrich.

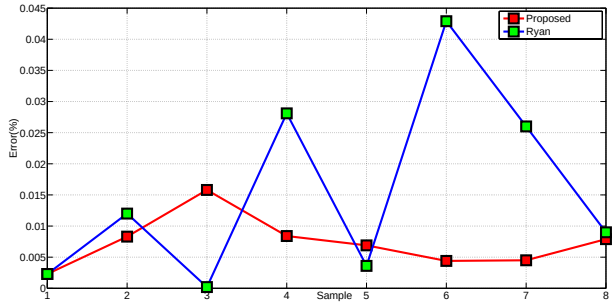

Figure 9. Details of comparative information between our proposed algorithm and Ryan.

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