Master's Thesis of Physics

Analysis of Raman spectra using denoising autoencoder

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Abstract

In many experiments, several denoising techniques are generally used to improve signal to noise ratio (SNR), such as averaging, filtering, smoothing and FFT/wavelet based algorithms. In particular, many studies have recently been conducted to apply learning-based methods such as denoising autoencoder (DAE) to denoising in experiments. Raman spectroscopy is a major experimental method that can study the internal structure and properties of molecules using Raman scattering. Especially, TERS (Tip-enhanced Raman spectroscopy) uses sharp tips to make reaction only near a point, enabling more accurate Raman signal analysis. However, in many experimental condition, SNR is often bad because Raman scattering occurs weakly. In order to increase SNR in Raman experiments, data is averaged through experimental iterations and analysis is carried out using Savitzky-Golay (S-G) smoothing. In the case of TERS, however, the repetition of long experiments is not good for experiment stability or cost issues because it makes the tip unstable. There is also a problem that S-G smoothing could erase important information corresponding to the weak signal of the Raman spectrum. In this paper, to solve the above problems, the two methods of applying DAE to the TERS experiment are presented using bulk water example. First, we made DAE learn data that is difficult to conduct S-G smoothing due to low SNR and confirmed that it can restore signals corresponding to ground truth without loss of information. Second, we made DAE learn data before and after averaging and confirmed that it could restore the averaging data with only a small portion of the data before averaging. This can increase the life of the tip and stability of the experiment by reducing the repetition of the experiment. This experiment has been applied to a well-known data sets such as bulk water signals, but it is expected that the same methodology can be applied to new experimental data to further enhance the quality of the TERS experiment.

Keyword : denoising autoencoder, Tip-enhanced Raman spectroscopy, bulk water
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Analysis of Raman spectra using denoising autoencoder*

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In many experiments, several denoising techniques are generally used to improve signal to noise ratio (SNR), such as averaging, filtering, smoothing and FFT/wavelet based algorithms. In particular, many studies have recently been conducted to apply learning-based methods such as denoising autoencoder (DAE) to denoising in experiments. Raman spectroscopy is a major experimental method that can study the internal structure and properties of molecules using Raman scattering. Especially, TERS (Tip-enhanced Raman spectroscopy) uses sharp tips to make reaction only near a point, enabling more accurate Raman signal analysis. However, in many experimental condition, SNR is often bad because Raman scattering occurs weakly. In order to increase SNR in Raman experiments, data is averaged through experimental iterations and analysis is carried out using Savitzky-Golay (S-G) smoothing. In the case of TERS, however, the repetition of long experiments is not good for experiment stability or cost issues because it makes the tip unstable. There is also a problem that S-G smoothing could erase important information corresponding to the weak signal of the Raman spectrum. In this paper, to solve the above problems, the two methods of applying DAE to the TERS experiment are presented using bulk water example. First, we made DAE learn data that is difficult to conduct S-G smoothing due to low SNR and confirmed that it can restore signals corresponding to ground truth without loss of information. Second, we made DAE learn data before and after averaging and confirmed that it could restore the averaging data with only a small portion of the data before averaging. This can increase the life of the tip and stability of the experiment by reducing the repetition of the experiment. This experiment has been applied to a well-known data sets such as bulk water signals, but it is expected that the same methodology can be applied to new experimental data to further enhance the quality of the TERS experiment.

Keywords: denoising autoencoder, Tip-enhanced Raman spectroscopy, bulk water

I. INTRODUCTION

Denoising has always been an important issue in data analysis, as it is impossible to completely eliminate noise environmentally in most scientific experiments. Conventionally, data has been denoised by statistical method such as averaging, or by various spatial domain filtering/smoothing([1]-[6]) method, FFT/wavelet based algorithm([7]), regularization, sparse representation algorithms or some other methods. Recently, learning-based denoising algorithm has been developed and utilized with the remarkable development of deep learning ([12]-[14]). Learning-based algorithm usually requires a lot of data and more complex architectures, but more accurate and robust denoising can be performed.

Among deep learning models, denoising autoencoder(DAE) is commonly used for denoising and has been successfully performed in many areas ([15], [16]). DAE is a neural network that learn with noisy data as input and clean data as output. In general, symmetrically with respect to the latent layer, the number of layers decreases as the layer gets deeper, and the number of layers increases again as it approaches the output layer(See Fig. 1). By this structure, the core features of the data set are encoded in the latent layer. Since the core feature of the data set follows the signal rather than noise, only the signal is restored during decoding to the output layer and denoising is successfully performed.

Even if there is no clean data, it was confirmed that high-quality denoising can be performed by learning noisy data by itself ([17], [18]). In addition, using the

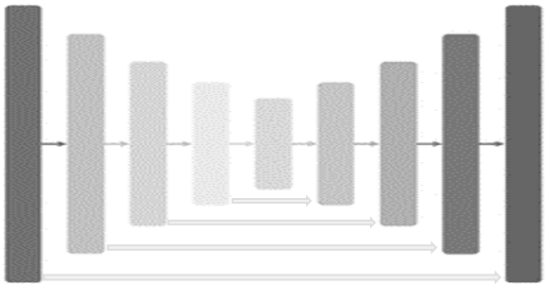

FIG. 1. Denoising autoencoder(DAE). It consists of an encoder that the number of layers decreases, a decoder that the number of layers increases and a latent layer on the center of network. The encoder extracts the key features of data and displays them in the latent layer. In the decoder, data is restored from the key feature again. As the number of data increases, denoising is naturally performed because the core feature represents the characteristic of the signal rather than noise. As the depth of the layer increases, the details of the input data may be lost, so the encoder and the decoder are symmetrically connected through a skip-symmetric connection not to lose details.

* A footnote to the article title
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properties of DAE, a methodology for fast obtaining physical quantities conventionally obtained over a long period of time in simulation or experiment was proposed ([19], [20]). These properties can be used in various physics experiments and data analysis.

Raman spectroscopy is an experimental methodology that analyzes the properties of molecules using Raman scattering. In particular, Tip-enhanced Raman spectroscopy(TERS) is an experiment that enables more precise analysis by enhancing the field near the tip using a small tip of the nm-scale ([21]). However, because a tip is smaller than the focused beam radius, the tip is easily damaged and it is still a challenging issue to conduct TERS without much damaging on the tip ([22]). Raman data analysis is performed by obtaining a graph of the intensity of light according to frequency as a measurement result and generally applying a baseline correction algorithm and Savizky-Golay smoothing for denoising on the results([23]).

In this paper, we present a data analysis methodology applicable to Raman or TERS experiments using DAE. Using the Raman spectrum of bulk water as an example, it was shown that DAE can achieve the same SNR of a large data set only using a small data set. From this, it is possible to minimize the damage to the tip by reducing the number of repetition of the experiment. In addition, it was confirmed that the DAE can produce same results as S-G smoothing by learning Raman data sets. S-G smoothing can be used for automation or double check for parameter selection because there is a degree of freedom for parameters.

II. BACKGROUND KNOWLEDGE

A. Denoising autoencoder([15])

Autoencoder is a kind of unsupervised-learning neural network that learns unlabeled data. Autoencoder is a network that connects an encoder and a decoder, and through these two processes, it learns a transformation close to an identity function. At this time, in the latent layer, which is the result of encoding, the input data is transformed in an appropriate hidden representation. For input data x_n

$$\begin{aligned} z_i &= decoder(encoder(x(i))) \\ &= decoder(y(i)) \\ &= x(i)(identity) \end{aligned}$$

Input x $\in$ [0,1] is encoded into the hidden representation

$$y = s(Wx + b)$$

through the encoder. s represents an arbitrary nonlinear fuction. Hidden representation y is reconstructed to

$$z = s(W'y + b')$$

through the decoder. At this time, the training is performed to minimize the reconstruction loss function by optimizing the parameters θ = (W, W′, b, b′).

In the denoising autoencoder, the training proceeds with corrupted data $\tilde{x} = x + noise$ as input and clean data x as output. In particular, when the latent layer is smaller than the input/output layer, the hidden layer removes noise by extracting a key feature of data, which is usually the signal. This allows the network to learn how to recover clean data from corrupted data.

Stacked denoising autoencoder is used to increase the quality of denoising or to perform blind denoising where clean data does not exist. For encoding layer $y^1, \ldots, y^n$ and decoding layer $z^1, \ldots, z^n$,

$$output\, z_i = z^n(...(z^1(y^1(\ldots(y^n(x_i))))))$$

In the case of a stacked autoencoder, when the depth of the layer becomes deep, it is difficult to learn because network forgets the details of the input data. To compensate for this, a skip-symmetric structure is usually added.

$$output\, z_i = z^n(...(z^1(y^1(\ldots(y^n(x_i)))) + y^1)) + y^n$$

B. Raman spectra([23])

Raman spectroscopy is a powerful technique for analyzing materials using Raman scaatering. A material has its own emission wavelength depending on its internal structure, and by measuring it, the internal structure can be inferred. But sometimes this is difficult because of the background signal and noise. Therefore, several methods have been studied to reduce background noise in Raman spectroscopy.

Background noise is composed of sample-dependent noise and detector-dependent noise. Sample-dependent noise includes changes in the internal structure of the sample due to environmental changes such as temperature and humidity, vibration of optical systems, and fluorescence of binding materials. detector-dependent noise includes an error in the CCD detector. In addition to this, there are errors due to the drift of used laser or external light source. It is generally known that sample-dependent noise is greater than detector-dependent noise.

In general, baseline correction is used to remove the background. Baseline correction is performed by minimizing the following loss functions for noisy original data y and smoothed data z.

$$S(z) = (y - z)^T(y - z) + \lambda z^T D^T D z$$

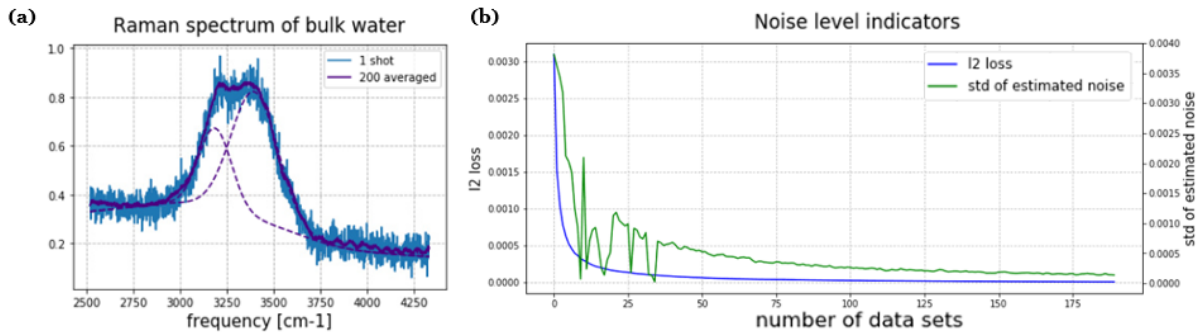

FIG. 2. (a) Raman spectrum of bulk water. Unsurprisingly, the noise is reduced when averaged. It is known that two peaks appear in the Raman signal of bulk water at room temperature and atmospheric pressure. When fitting with two gaussians after baseline correction, the above result appears. (b) noise level indicators according to the number of data sets used for averaging. The blue line is L2 loss to averaged data of 200 sheets according to the number of data sets used for averaging. Since the average of 200 sheets is taken as the ground truth, it converges to zero. Actually, the average of 200 sheets is not ground truth, so noise still exists even if it reaches 0. The green line is single-image noise level estimation result according to the number of data sets used for averaging. We used an algorithm that roughly estimates the noise level by dividing the data by patch units. If the data is small, the noise is high and accurate calculation cannot performed. If one uses beyond 120 sheets, one can see that it no longer decreases.

$$D = \begin{pmatrix} 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 \end{pmatrix}$$

The first term is a mean-squared error term that allows smoothed data to follow the trend of the original data. The second term is a smoothing term that uses matrix D to bring the data closer to the average of the points on both sides. At this time, by adjusting the lambda, you can draw a smoothed line that follows the trend of data as much as you want.

$$S(z) = (y - z)^T W (y - z) + \lambda z^T D^T D z$$

$$W = \begin{cases} +w & \text{if } y > z \\ -w & \text{if } y < z. \end{cases}$$

The baseline can be found by adding the W matrix to the first term. W is determined by the difference of y and z, moving the smoothed line up or down. Selecting a smoothed line that follows the baseline well through appropriate selection of w and lambda, background signal can be removed by subtracting it from the original data.

Raman spectra's denoising generally uses Savizky-Golay smoothing. S-G smoothing is a smoothing method that replaces $\tilde{x}$ with x by interpolating the points included in the window around the given point $\tilde{x}$ to the nth order polynomial. Each interpolation takes much time to calculate, but it is knouwn that one can replace this process with a convolutional algorithm. S-G smoothing is fast and perform noise reduction well depending on the choice of parameters, so it is still widely used in Raman spectrum analysis. However, the parameters is selected only by background knowledge and human sense, so there are problems in reliability and automation.

III. EXPERIMENTAL SETUP

A. Data sets

For the experiment, the Raman spectrum of the bulk water sample was measured. The experiment was conducted at room temperature and atmospheric pressure, and measurements were conducted by dropping a bulk water sample on a silicon plate. The monochromator

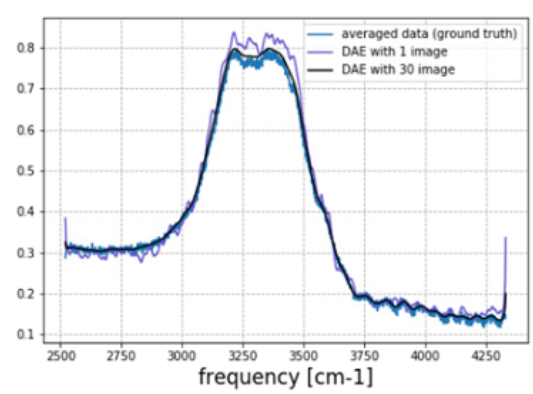

FIG. 3. DAE results of test set. When using 1 sheet of data as DAE input, there is a large error to the ground truth. When using 30 sheets, one can see that the result is similar to the ground truth.

used for the measurement was DongWooDM150i, and the grating was set to 600/500nm. The exposure time of each experiment was 0.5ms, and 50 sets were prepared with 200 experiments as one set.

B. DAE specification

The specifications of the DAE used in the experiment are as follows (See Fig. 1). It consists of four layers of encoders and four layers of decoder, each of which consists of a pair of 1d convert layer and a pooling/upsampling layer. For convolutional layer, the kernel size is 5 and the activation function is "elu" and consisting of 256, 128, 64, 32 filters per each layers. The stride of pooling/upsampling is 2, and the dropout after pooling/upsampling is 0.2. Using symmetric skip connection to conserve details of input data.

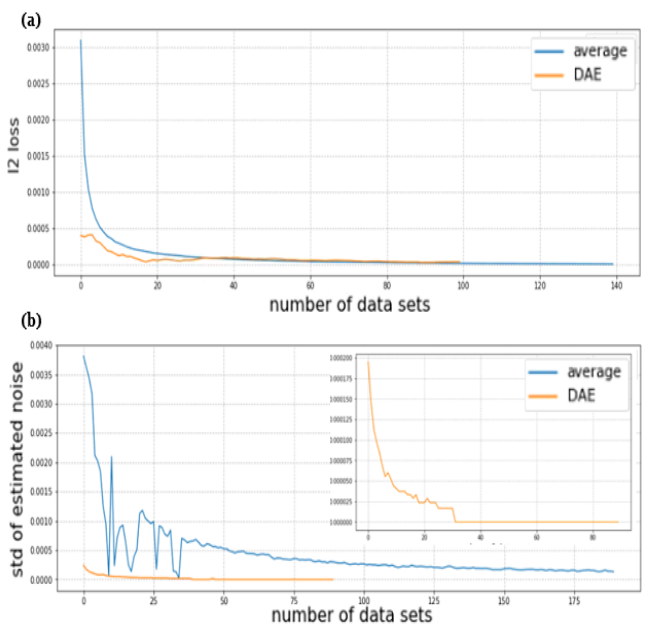

FIG. 4. (a) L2 loss to averaged data of 200 sheets according to the number of data sets used for averaging or DAE input. With less than 20 sheets of data, it can be seen that l2 loss is measured similar to the result of averaging more than 80 sheets. In the case of the DAE result, even if the number of data increases, it does not converge to 0 because the reference point of l2 loss is set to the average data of 200 sheets, but it is not a real ground truth. Although there is an inaccuracy of the indicator, it is clear that a high SNR can be obtained with less data. (b) noise level estimation according to the number of data sets used for averaging or DAE input. As can be seen in <Fig. 3>, DAE shows very low noise level because there is almost no noisy vibration in patch units of DAE results.

IV. RESULT

A. Averaging

In order to compare with the conventional methodology and confirm the motivation of this paper, the denoising power of averaging according to the number of data was calculated. L2 loss to averaged data of 200 shots and single-image noise level estimation algorithm ([24]) were used as indicators to calculate it. The results are shown in <Fig. 2>.

Looking at the results, it can be seen that when the number of data exceeds about 100, there is no advantage in repeating the experiment. We can get the two motivations from this. The first is to obtain the same level of SNR by using a smaller amount of data instead of obtaining the maximum SNR by averaging 100 sheets. As mentioned above, repetition of the experiment damages the tip and thus declines the accuracy and stability of the experiment. Therefore, obtaining a high SNR using a small amount of data can help the stability and cost reduction of the experiment. The second is to obtain a result that exceeds the maximum SNR obtained by averaging of 100 sheets. Conventionally, this task is performed using S-G smoothing, but this is insufficient because there is a degree of freedom in parameter selection. Using DAE, one can efficiently compensate the

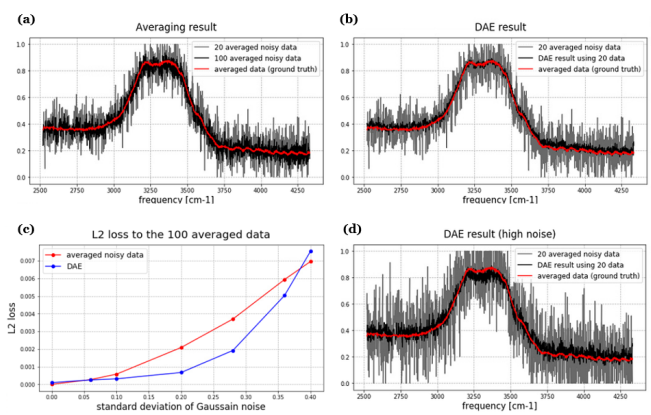

FIG. 5. (a) Experimental data with Gaussian noise ($\sigma = 0.2$) added. The gray line is the averaged data of 20 sheets and the black line is the averaged data of 100 sheets. The error is large compared to the original data. (b) Results of DAE using the 20 data sheets. The denoising quality is not good compared to the result without adding noise, but it can be seen that the result was much better than the average of 100 sheets(a). It could help shorten the actual experiment. (c) L2 loss according to noise amplitude. Up to a certain range, it can be seen that the DAE produces good results more than the average of 100 sheets. If it exceeds $\sigma = 0.4$, the quality of denoising decreases. (d) DAE result when $\sigma = 0.4$. In particular, it is confirmed that the signal part is shifted downward and does not fit well. If the noise exceeds a certain level, the performance of the DAE is degraded.

shortcomings of S-G smoothing.

B. Speed up

Denoising autoencoder learns how to extract clean data from noisy data by inputting noisy data and outputting clean data. Assuming averaged data of 100 sheets as clean data, and averaged data of 1-99 sheets as noisy data to it, DAE can learn how to get 100-sheets-averaged out of a small number of data. Using the example data obtained from bulk water, we made DAE learn the averaged data of 1-99 sheets to the data averaged 100 sheets each. After training, the test set was used to confirm the results as shown in <Fig. 3>.

The result of calculating the noise level according to the number of data can be checked in <fig. 4>. Looking at the results, it can be seen that from the DAE results with 20 data sets or less, the same or better results can be obtained than the simple averaging of 80 data sets or more. Since the average of 100 or 200 sheets is not the actual ground truth, there is an inaccuracy of the indicator itself, but it is certain that DAE can produce sufficiently meaningful results from a small amount of data. This can help increase the life time of the tip and increase the stability of the experiment by reducing the repetition of the experiment, especially in the TERS experiment.

In the case of the bulk water experiment results, the SNR is high enough, so there is no problem in data analysis even if fitting is performed without using a large amount of data. Therefore, if the SNR is high, it is doubtful that DAE can reduce experiment repetitions. To test the case where the SNR is low and analysis is possible only when a large amount of data is used, simulation noise was added to the experimental data to confirm whether the DAE can give a meaningful result. The added noise is Gaussian noise, and the analysis was carried out by increasing the standard deviation σ.

In <Fig. 5>, one can check the DAE result when the SNR is lowered. It can be seen that if $\sigma = 0.4$ or more, the reliability of the result is poor. When referring to existing studies on image denoising, it is expected that DAE can be applied even to higher noise, but in this experiment, the number of data was limited, so no better results could be achieved. Actual experiments also have limitations in obtaining a lot of data, so using a lot of data will be limited.

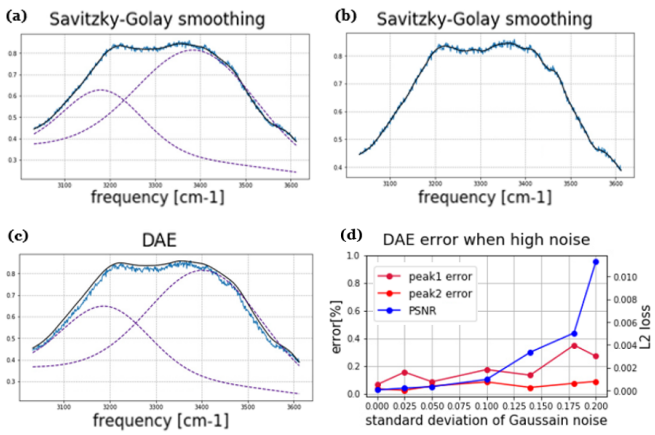

FIG. 6. (a), (b) S-G smoothing results. Depending on the parameter selection, one can see 2(a) or 5(b) peaks. The only criterion for choosing the right outcome is human background knowledge. (c) DAE result. Compared to S-G smoothing, it looks slightly out of the data trend. However, the positions of the peak are 0.065, 0.034% different for S-G smoothing, respectively, and the amplitude ratio is 1.1% different for it. In the case of amplitude, it changes according to the baseline correction parameters. So relatively large difference of amplitude is due to this, and even considering this, DAE result can be seen as a sufficiently similar result with S-G smoothing. The reason the DAE result is shifted upward is because the overall data distribution of training set is shifted upward. (d) The result of DAE learning when adding Gaussian noise. It learns without clean data, so the L2 loss increases with less noise than the former case. In the case of the positions of the peaks, the error does not increase much because the existence of two peaks were already known. If the noise increases and denoising is not done properly, it will be difficult to be sure if the two peaks exist without background knowledge.

C. High SNR

As mentioned in the Introduction, Denoising autoencoder can learn denoising methods by learning noisy data on itself. One cannot obtain better clean data than the noisy data of 100 sheets average, so DAE learned 100-average data by itself. Learning results are shown in <Fig. 6>.

Due to the baseline correction error, there is a slight difference in the ratio of amplitude, but it can be seen that the result is almost similar to S-G smoothing. As can be seen in <Fig. 6>, S-G smoothing has a degree of freedom of parameters, and the criterion for selecting a better result is only human subjective judgment based on background knowledge. The DAE result can also produce different results depending on the hyperparameters, but since it can be quantified by the loss function, a hyper-

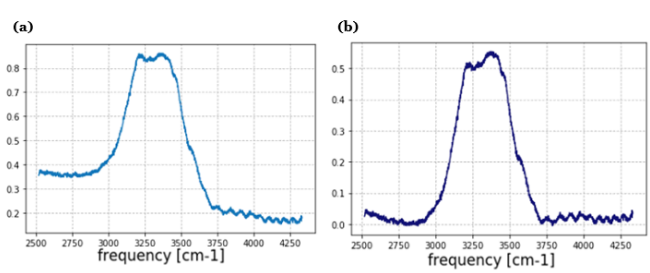

FIG. 7. (a) Raman spectrum of bulk water. (b) baseline correction result of (a).

parameter with a low loss can be selected. Through this, DAE can help in parameter selection of S-G smoothing or be used as a substitute for S-G smoothing, or it can be utilized as automation of smoothing because human selection process can be omitted.

V. CONCLUSION

We present an efficient methodology for analysis of Raman spectra using Denoising Auto Encoder. First, DAE learning helped us to get close results to averaging data of 100 shots with about 20 shots. The life time of the tip and the stability of the experiment can be increased by reducing the number of repetition of the experiment. Second, DAE learning was used to achieve similar results with SG smoothing. It can be used for automation of smoothing and double check of SG smoothing.

For future work, we are planning the following experiments. The measured Raman data is usually shifted upwards by background noise (See Fig. 7). To correct this, the baseline correction algorithm is conventionally used. We plan to confirm that not only S-G smoothing but also baseline correction can be replaced by DAE by learning original data as input and baseline correction result as output.

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