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Denoising scheme based on singular-value decomposition for one-dimensional spectra and its application in precision storage-ring mass spectrometry

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This work concerns noise reduction for one-dimensional spectra in the case that the signal is corrupted by an additive white noise. The proposed method starts with mapping the noisy spectrum to a partial circulant matrix. In virtue of singular-value decomposition of the matrix, components belonging to the signal are determined by inspecting the total variations of left singular vectors. Afterwards, a smoothed spectrum is reconstructed from the low-rank approximation of the matrix consisting of the signal components only. The denoising effect of the proposed method is shown to be highly competitive among other existing nonparametric methods, including moving average, wavelet shrinkage, and total variation. Furthermore, its applicable scenarios in precision storage-ring mass spectrometry are demonstrated to be rather diverse and appealing.

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I. INTRODUCTION

Noise is ubiquitous in the outcome of any physical experiment, owing to statistical fluctuations and various uncontrollable disturbances affecting the measuring system. It is superposed over the measured signal and obscures the inference of the underlying ground truth. To reduce the noise effect, usually a batch of independent measurements under the same condition are performed for averaging, since the noise variance scales inversely with the averaging number. However, the accumulated statistics may be insufficient to bring down the noise due to pragmatic constraints. Or even the measurement is just a one-shot instance. Under those circumstances, data denoising in the later analysis can only be resorted to as a mitigation.

It is quite common that measurement results are encoded in one-dimensional spectra, such as the energy spectrum of a γ -radioactive isotope, the frequency response of a notch filter, or the hourly temperature readings of a thermometer. Mathematically speaking, it is an ordered sequence of real-valued numbers, where usually the signal is smooth while the noise overlays complex irregularities like kinks and wiggles. In this sense, smoothing can be used interchangeably with denoising in the context of one-dimensional data analysis.

Despite the voluminous data smoothing techniques, there are in general two categories, namely, parametric and nonparametric. A parametric method starts with a data model built from *a priori* knowledge on the signal and the noise. Such knowledge can be a theoretical comprehension of the measuring system or merely an educated guess. In contrast, a nonparametric method makes a minimal assumption about the noise and then lets the data speak for themselves. Thus with

less restrictions, nonparametric methods own more versatility and applicability.

As an example in the nonparametric category, moving average probably is the most intuitive method [1]. The smoothed sequence is formed by replacing every noisy datum with the (weighted) mean of data in its neighborhood. This is essentially equivalent to convolution smoothing [2], where the noisy sequence is convolved with a smoothing kernel such as binomial, Gaussian, or exponential [3]. In the same vein, the neighborhood for averaging can be extended to encompass data with similar values, which has inspired two other methods: bilateral filter [4] and nonlocal means [5].

When viewed from a different perspective, the convolution smoothing is in fact low-pass filtering in the Fourier-transformed domain [6], where the smoothing kernel is the impulse response of the filter. Normally the signal is band-limited whereas the noise covers the whole domain, hence a low-pass filter can effectively reject most of the noise. Based on the same Fourier transform, another method named Fourier thresholding takes a different approach to data denoising [7]. It abandons sinusoidal components whose transform coefficients are below a given threshold, as they more likely belong to the noise.

Like Fourier transform, wavelet transform is another powerful tool in digital signal processing [8], which decomposes an input sequence into localized oscillatory components. The Fourier-based data denoising methods can likewise be migrated to the wavelet-transformed domain. As a counterpart of the Fourier thresholding, wavelet shrinkage manipulates wavelet coefficients according to a specific criterion to smooth a noisy sequence [9,10].

Lastly, it is worth noting a special mainstream method in the nonparametric category: total variation regularization [11], whose underlying framework differs from the aforementioned. The idea is to minimize the total variation, which is

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the ℓ_1 -norm of its first derivative, of the smoothed sequence. Meanwhile, it also tries to preserve data fidelity as the regularizing condition. Since the ℓ_1 - rather than ℓ_2 -norm is adopted, this method is good at retaining discontinuities in the noisy sequence [12], but also suffers from a staircase effect in the smoothed one [13].

On the contrary, curve fitting of a predefined signal model by least-squares regression is a typical data de-noising example in the parametric category. To apply the fitting, the noisy sequence can be treated as a whole or in partitions, where the latter gives rise to locally weighted regression [14] and Savitzky-Golay filter [15]. If additionally a noise model is defined, then data denoising can be achieved in a more sophisticated manner. Examples are Wiener filter [16] and Kalman filter [17], which are both rooted in statistical inference and estimation.

In the work presented here, we propose a nonparametric one-dimensional data denoising method based on singular-value decomposition (SVD). The SVD is a well-developed matrix factorization technique [18], which can be used to realize the idea of principal component analysis [19]. Its applications are prevalent in digital signal processing, especially in two-dimensional image-related works such as coding, watermarking, and denoising [20–23]. With the aid of a bijective map from a sequence to a matrix, the SVD also plays a role in one-dimensional data analysis, such as speech recognition [24], fetal electrocardiogram extraction [25], mass spectrometry [26], and fault diagnosis in mechanical systems [27–30]. In particular for the data denoising, a noisy sequence is to be decomposed by SVD, where a smoothed sequence can be reconstructed from a selected subset of the components.

II. METHOD

Let us consider a noise-corrupted sequence x of length n , which consists of the signal a and the noise d :

$$x_i = a_i + d_i, \quad 0 \leq i < n. \quad (1)$$

Here, we have made no assumptions about the noise other than being additive, zero-mean, and white.

The proposed data denoising method mainly includes three steps: (1) Embed the sequence into a matrix. (2) Apply SVD to the matrix and determine signal components. (3) Reconstruct a smoothed sequence with the selected components. In the following, each step will be elaborated.

A. Matrix selection

In literature there are mainly three approaches to embed the sequence x into a matrix. Probably the simplest one is to evenly partition x into segments, which are then stacked to form a matrix [25,27,31]. This approach is mostly suitable for a quasi-periodic sequence, when each segment roughly contains one or multiple periods. Another approach is to build a time-frequency representation of x [32], which can be computationally expensive. As a matter of fact, the frequently adopted approach is to construct a Hankel matrix [24,26,28–30,33,34], which balances algorithmic performance and computational cost.

FIG. 1. Illustration of different denoising effects with two matrix-embedding approaches. (a) The green line shows the denoised result with a Hankel matrix, while the blue line corresponds to a partial circulant matrix. The orange line is the ground truth. (b) Deviations of the two results with respect to the ground truth.

Specifically, the constructed Hankel matrix H of size $m \times (n - m + 1)$ reads

$$H_{ij} = x_{i+j}, \quad 0 \leq i < m; 0 \leq j \leq n - m. \quad (2)$$

Apparently, the choice of m will somehow influence the smoothing effect. It is shown that m should best be $n/2$ or $(n + 1)/2$, depending on the parity of n [29]. That is to say, H should optimally be (almost) square.

However, a drawback of the mapping in Eq. (2), which is often overlooked, is that the elements of x are not put on an equal footing, i.e., the central elements tend to occur more times in H than the lateral ones. Numerical experiments have proved that by construction of H the signal details close to the sequence ends can badly be recovered after denoising.

Figure 1 illustrates such a phenomenon with a synthetic sequence, which is the superposition of a sinc signal and a normal noise. The sequence of length $n = 1000$ is embedded into H with a row number $m = 500$. It is evident that the denoised sequence (see green line in Fig. 1) strongly deviates from the ground truth (see orange line in Fig. 1) at both ends, where the largest deviation amounts to 10.5%. What is worse, the deviation is so large that the denoised sequence is notably off the noisy one, which indicates the inability to respect lateral information in the case of denoising with H .

To overcome this limitation, we thus propose to construct a partial circulant matrix X of size $m \times n$ with $m \leq n$:

$$X_{ij} = x_{(i+j) \bmod n}, \quad 0 \leq i < m; 0 \leq j < n. \quad (3)$$

Every row of X is a cyclic left-shift of the above one by an element, such that every x_i occurs exactly m times. By virtue of X with the same row number $m = 500$, the denoised sequence, which is shown with the blue line in Fig. 1, resembles more the ground truth, and the overall deviation is within 2.3%. Moreover, the denoised sequence tends to turn

FIG. 2. Typical examples of SVD components in the case of noise-corrupted signal (left), sole signal (center), and sole noise (right). (a1) Full spectra of singular values in a nonincreasing order, where the blue crosses belong to the signal and the green dots belong to the noise. (a2) similar to (a1), but for sole signal; (a3) similar to (a1), but for sole noise. (b1) Zoomed spectra focusing on the largest six singular values. (b2) similar to (b1), but for sole signal; (b3) similar to (b1), but for sole noise. (c1) The corresponding left singular vectors. (c2) similar to (c1), but for sole signal; (c3) similar to (c1), but for sole noise.

back to the ground truth at both ends, which is in contrast to the previous tendency as a result of denoising with H .

B. Low-rank approximation

For the matrix X defined in Eq. (3), the Eckart-Young theorem has asserted that it can be decomposed to (at most) m rank-one matrices [35]:

$$X = \sum_{i=0}^{m-1} s_i \mathbf{u}_i \mathbf{v}_i^T, \quad (4)$$

where the singular values s_i are nonnegative and ordered nonincreasingly; the left singular vectors $\mathbf{u}_i \in \mathbb{R}^{m \times 1}$ are orthonormal; and similarly for the right singular vectors $\mathbf{v}_i \in \mathbb{R}^{n \times 1}$. When expressed with matrix notation, Eq. (4) leads to the canonical form of SVD:

$$X = U \Sigma V^T, \quad (5)$$

where Σ is an $m \times m$ diagonal matrix composed of s_i as the nonzero elements; U is an $m \times m$ matrix composed of $\mathbf{u}_i$ as the column vectors, while V is an $n \times m$ matrix composed of $\mathbf{v}_i$.

The physical interpretation for s is that each element describes the amount of energy distributed in the corresponding component. Specifically, the total energy of x is proportional to the squared Frobenius norm of X :

$$\|X\|_F^2 = \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} X_{ij}^2 = m \sum_{i=0}^{n-1} x_i^2. \quad (6)$$

Meanwhile, by Eq. (5), $\|X\|_F^2$ can be written as

$$\|X\|_F^2 = \text{trace}(X^T X) = \text{trace}(\Sigma^2) = \sum_{i=0}^{m-1} s_i^2. \quad (7)$$

Since s is nonnegative and nonincreasing, by selecting the largest r singular values and setting the remaining s_i to zero, the resultant matrix A is the best rank- r approximation of X in terms of minimizing the approximation error energy [35]. This sets the theoretical basis for the data denoising method

proposed here. In practice, most of the singular values are close to zero [see Fig. 2(a1) for illustration], which can be attributed to the noise. Therefore, X can be well approximated with a few predominant signal components only.

That said, one question remains to be answered: Which index separates the signal components from the noise ones? Despite different solutions in literature, it is certainly impossible to agree on a universal approach that fits in every realistic situation and fulfills every practical requirement.

Nevertheless, a majority of the methods choose to look into the intrinsic structure of the singular values, or its variants like singular entropy [29,36], to search for the “elbow point” in Fig. 2(a1). To name a few, one can inspect the first-order difference [29,32], the first-order quotient [27,30], or simply select the intersection of two extrapolated lines by eye [31]. All those methods depend on extra deciding parameters, which are usually specified *ad hoc* and vary from case to case. Consequently, it is rather difficult to implement them in an automated manner to denoise a large batch of sequences. What is worse, the smoothed sequence is prone to subjective bias, and thus may vary from person to person.

A more advanced method seeks to approximate X when regularized by the nuclear norm of the low-rank approximator [23,37]. To select an appropriate regularization parameter, this method relies on various unbiased risk estimators according to the prior knowledge on the noise statistics. Other sophisticated methods based on neural network dictionary learning require considerable training data, and often involve many iterations to solve nonlinear minimization problems [25,33]. Apparently, those methods are computationally rather intense.

Here, we propose to tackle this challenge by inspecting the left singular vectors. As can be seen in Fig. 2(c1), the first three belonging to the signal are quite smooth, whereas the noise vectors are very wiggly. Moreover, there exists a drastic behavioral change at the critical index, which separates the signal from the noise. This observation is further confirmed by Figs. 2(c2) and 2(c3), where the signal and the noise are individually inspected. To characterize such an impression, a quantity named normalized mean total variation (NMTV) is defined. For a given sequence w of length m , the NMTV ξ is

calculated as

$$\xi = \frac{\sum_{i=0}^{m-2} |w_i - w_{i+1}|}{(m-1)(w_{\max} - w_{\min})}. \quad (8)$$

Obviously, ξ is between zero and one, where zero means no variation and one corresponds to a zigzag pattern. A larger NMTV indicates that the sequence is more oscillatory. Hence, the NMTV is able to describe the smoothness of the sequence. Since the noise is usually wiggly, its SVD components can be discriminated by thresholding on the NMTVs of $\mathbf{u}_i$. Numerical experiments have revealed that a universal threshold of 0.1 should be suitable in most, if not all, cases.

C. Signal reconstruction

Having selected the first r SVD components, the low-rank approximation A of X is

$$A = \sum_{i=0}^{r-1} s_i \mathbf{u}_i \mathbf{v}_i^T. \quad (9)$$

In general, A is no longer partially circulant. Consequently, cyclic antidiagonal averaging is applied to reconstruct the smoothed sequence $\hat{a}$ from A :

$$\hat{a}_i = \text{mean}_{j+k \equiv i \pmod{n}} (A_{jk}), \quad 0 \leq i < n. \quad (10)$$

D. Practical considerations

So far, the choice of m has not been addressed. It is nevertheless worth noting that when $m = n$, i.e., X is completely circulant, the method proposed here is equivalent to the Fourier thresholding [7]. Since any circulant matrix is diagonalizable by the unitary discrete Fourier transform matrix, its singular values obtained by SVD are in fact the modulus of the Fourier coefficients of x [38].

However, to select a larger m does not necessarily result in a better smoothing effect, as the signal energy is diluted by excessive singular values. A relatively small m is not much helpful either due to an insufficient number of elements for the cyclic antidiagonal averaging. Although in practice the choice of m may be subject to the specific purpose of the denoising problem, one can generally decide on an optimal m which minimizes the NMTV of the denoised sequence to attain the smoothest result. Numerical experiments have suggested an empirical rule to achieve an optimal denoising effect: $0.1n < m < 0.4n$.

Sometimes, it will be unfortunate to notice a ringing artifact in the smoothed data, in particular when the signal has a significant gap between its two ends (Fig. 3). This should be owing to the same reason as for the Gibbs phenomenon in Fourier transform [39]. As a cure for the artifact, a linear trend, if at all, in the signal should be removed to close the gap before denoising. Whether the detrending is practically necessary is judged by a comparison between the signal gap Δ and the noise standard deviation σ .

Unfortunately, neither of them are known, and hence they must be estimated from x . Despite the wiggles at both ends of x , the respective signal end-values can be recovered somehow by averaging a few neighboring data, based on which Δ is estimated. Moreover, σ can be estimated from the noise

FIG. 3. Illustration of the ringing artifact in the smoothed data. The blue line is obtained with linear detrending, whereas the green line without.

singular values. By recalling Eqs. (1), (6), and (7), it can be written that

$$\sum_{i=0}^{n-1} a_i^2 + \sum_{i=0}^{n-1} d_i^2 + 2 \sum_{i=0}^{n-1} a_i d_i = \frac{1}{m} \sum_{i=0}^{r-1} s_i^2 + \frac{1}{m} \sum_{i=r}^{m-1} s_i^2, \quad (11)$$

where, due to the cancellation among d_i , the summation of the cross terms on the left side contributes rather little. Therefore, σ can be approximated as

$$\sigma = \sqrt{\frac{\sum_{i=0}^{n-1} d_i^2}{n}} \approx \sqrt{\frac{\sum_{i=r}^{m-1} s_i^2}{mn}}. \quad (12)$$

Should σ turn out to be less than Δ after denoising, a linear trend is significantly present and must be removed. However, it may happen sometimes that for the detrended yet noisy sequence, σ is still less than Δ , which suggests that the estimate of the latter by averaging is strongly biased by the signal itself. Under such circumstances, it is advisable to reduce the number of elements for averaging and redo the detrending. This adaptive detrending process will surely terminate, in the worst case, when the averaging number becomes one.

In summary, the algorithm of the proposed data denoising method is organized as follows.

- (1) Begin with a noisy sequence x and a row number m .
- (2) Construct a partial circulant matrix X by Eq. (3), then apply SVD to it.
- (3) Calculate the NMTVs of the left singular vectors $\mathbf{u}_i$ by Eq. (8), then select the smallest r that satisfies $\text{NMTV}(\mathbf{u}_{r-1}) < 0.1 \leq \text{NMTV}(\mathbf{u}_r)$ as the approximation rank.
- (4) Estimate the signal gap Δ by averaging a few end-data in x , as well as the noise standard deviation σ by Eq. (12).
- (5) If $\sigma < \Delta$, linearly detrend x , then repeat steps (2)–(4); otherwise, proceed.
- (6) Build a low-rank approximation A by Eq. (9).
- (7) End with a smoothed sequence $\hat{a}$ by Eq. (10).

III. EXAMPLES

To illustrate the smoothing effect of the proposed method, four synthetic signals of the same length $n = 1000$ are adopted for test. They are intentionally selected to embody

FIG. 4. Illustration of the smoothing effect on the noise-corrupted periodic signals with various SNRs. (a) The noise obeys a uniform distribution. The orange line is the ground truth, while the blue line is the denoised approximation. (b) Same as (a), except the noise is normally distributed. (c) The resultant NRMSDs obtained in different cases.

different data traits that are frequently seen in practice. Specifically, their synthetic formulas are listed below, with $0 \leq i < 1000$.

Periodic signal:

$$a_i = \sin(0.004\pi i) - \sin^3(0.008\pi i) + \cos[\sin(0.008\pi i)], \quad (13)$$

which contains exactly two periods.

Asymmetric peak:

$$a_i = \text{erfc}(3 - 0.01i) \cdot e^{-0.01i}, \quad (14)$$

where $\text{erfc}(z) = 1 - \pi^{-1/2}(\int_{-z}^{\infty} e^{-t^2} dt)$ is the complementary error function.

Multiple peaks on a ramp:

$$a_i = e^{-(0.02i-6)^2} + [2 + (0.04i - 28)^2]^{-1} + e^{-0.001i}, \quad (15)$$

which contains a Gaussian peak and a Lorentzian peak.

Chaotic dynamics: It is well known that a Duffing oscillator will undergo chaos under certain conditions [40]. Here, we adopt the following parametrization of the Duffing equation:

$$\ddot{a} + 0.3\dot{a} - a(1 - a^2) = 0.5 \cos(0.4\pi t), \quad (16)$$

where a denotes the oscillation amplitude, and the dotted versions denote its derivatives with respect to time t . With the initial value $(a, \dot{a})_0 = (1, 0)$, the differential equation is numerically solved by the Runge-Kutta fourth-order method in an interval of $0 \leq t < 50$ with a resolution of 0.05.

The synthetic signals are then contaminated by adding respectively two types of noise, namely uniform and normal, to produce noisy sequences. The amount of the contamination is controlled by the signal-to-noise ratio (SNR) ranging from 0 to 20 dB, which is defined as

$$\rho_{\text{dB}} = 10 \log_{10} \left(\frac{\langle a^2 \rangle - \langle a \rangle^2}{\langle d^2 \rangle - \langle d \rangle^2} \right), \quad (17)$$

where $\langle \cdot \rangle$ denotes arithmetic mean. It is clear that a smaller ρ will lead to a more wiggly sequence.

A fixed row number $m = 250$ is selected for all the smoothing tests. The denoising goodness is assessed by the normalized root-mean-square deviation (NRMSD) of the smoothed sequence $\hat{a}$ from the signal a , which is defined as

$$\delta_{(\%) } = 100 \sqrt{\frac{\langle (\hat{a} - a)^2 \rangle}{\langle a^2 \rangle - \langle a \rangle^2}}. \quad (18)$$

A smaller δ indicates a greater power to reveal the ground truth.

FIG. 5. Same as described in the caption of Fig. 4, but for an asymmetric peak.

FIG. 6. Same as described in the caption of Fig. 4, but for a Gaussian peak (left) and a Lorentzian peak (right) on a ramp.

The test results are shown in Figs. 4–7. It can be seen that the proposed method is well able to smooth the noisy sequences, regardless of the underlying signals, even when the SNR is down to 0 dB. The achieved NRMSDs are quite similar for both types of noise, although the normal noise usually results in a slightly larger NRMSD, which may be owing to its larger kurtosis.

IV. APPLICATIONS

Owing to its nonparametric nature, the method presented here is promising to find its applications in vast data denoising scenarios. Furthermore, by allowing for a manual selection of the approximation rank, the proposed method will be a powerful data analysis technique not just for denoising. In what follows, three data analysis challenges in precision storage-ring mass spectrometry are presented to showcase its diverse applications in reality [41].

A. Pulse timing

In the isochronous mass spectrometry [42], a relativistic charged particle periodically circulates in a vacuum environment due to the confinement by magnetic field [43]. A time-of-flight detector consisting of an ultra thin carbon foil is placed in the vacuum chamber to register every passage of the particle, which is signaled by a sharp voltage pulse [44]. Fig. 8 shows a zoomed example of such a pulse. A

precise determination of the pulse onset is critically important for a high-precision (<1 ppm) mass measurement [45–47]. Unfortunately, due to thermal noise and quantization error, in particular for weak pulses, the pulse leading edge is distorted, which limits the timing accuracy. Furthermore, the voltage uncertainty in pulse samples also degrades the timing precision, since the leading edge can only have a nonzero fall time, which is the duration for the pulse to dive from 90% to 10% of its full depth. In general, a smaller fall time will result in a better timing precision. As for the timing accuracy, it can be improved by employing a competent data denoising technique.

With the same pulse of length $n = 401$ in Fig. 8, we have compared four denoising methods of nonparametric type, namely, the one proposed here, moving average, wavelet shrinkage, and total variation. The NMTVs of their denoised data, which are shown in Table I, are controlled to be almost the same to ensure comparable smoothness. Afterwards, the fall time is measured for each smoothed sequence, except for the total variation since the staircase effect unfeasibly allows for a clear definition of falling interval. In what follows, the technical implementing details are presented.

For the proposed method, a row number $m = 105$ is determined. As for the moving average, a Gaussian kernel g of length 45 and standard deviation 9 is employed:

$$g_i \propto e^{-i^2/162}, \quad -22 \leq i \leq 22. \quad (19)$$

FIG. 7. Same as described in the caption of Fig. 4, but for the amplitude of a Duffing oscillator.

FIG. 8. A zoomed pulse recorded by a time-of-flight detector, which is denoised by (a) the proposed method in this work, (b) moving average, (c) wavelet shrinkage, and (d) total variation. The crosses on the leading edge mark the 90% to 10% interval used to calculate the fall time. See Sec. IV A for the detail.

When applying the wavelet shrinkage, the Symlets-4 is adopted to perform the wavelet decomposition. Afterwards, the wavelet coefficients are thresholded on 3.406 using the nonnegative garrote scheme [48,49]. The wavelet transform is carried out in Python with the PyWavelets package [50]. Lastly, the total variation is based on the algorithm for one-dimensional data in Ref. [51], and computed with the C code available in Ref. [52]. The regularization parameter for total variation is selected to be 2.89.

The denoised results by these four methods are shown in Fig. 8, and the obtained fall times are listed in Table I. It is found that the proposed method produces the smallest fall time, which can in principle lead to the best timing precision. In contrast, the wide kernel of moving average not only leaves apparent vacancy in the denoised data at both ends, as pointed by arrows in Fig. 8(b), but also smears out the leading edge. The wavelet shrinkage superfluously causes a leading bump and trailing spikes, as pointed by arrows in Fig. 8(c), where the former also degrades the fall time. As for the total variation, the disturbing staircase effect, as shown in Fig. 8(d), makes it improper for accurate and precise pulse timing. It can therefore be concluded that by means of the proposed method, timing of weak pulses has become feasible with satisfactory accuracy and precision, thus relaxing the saturation constraint of the detector [53].

B. Prewhitening

In the Schottky mass spectrometry [54], a dedicated resonator is employed to detect a revolving particle in the storage ring by sensing its electromagnetic radiation [55]. Owing to

TABLE I. Characteristics of denoised data by various methods.

Method	NMTV (%)	Fall time (ns)
This work	5.70	0.38
Moving average	5.69	0.53
Wavelet shrinkage	5.71	0.51
Total variation	5.70	—

FIG. 9. Background estimation of a Schottky spectrum with a sharp peak on top of it. The blue line is a direct fitting of a Lorentzian function, whereas the red line is obtained by the proposed method in this work. The green line acts like a reference.

the periodic motion of the particle, the power spectral density of its Schottky signal detected by the resonator peaks at each harmonic of the particle's revolution frequency [56]. Among those harmonics, the one in the resonant range of the resonator is band-pass filtered and mixed down to the base band for data acquisition [57].

Figure 9 shows an example of a peak harmonic on top of a resonant background. In certain cases, the integral peak area is of the experimental interest, from which the particle number can be inferred [56,58]. This is a prior step for, e.g., the measurement of the particle's lifetime [59], or the calibration of the particle's position [60]. Therefore, a proper deduction of the background is of the experimental importance.

Although the Lorentzian shape of the background is well understood [61], it is improper to directly apply fitting to the spectrum as the peak will strongly deviate the result (see blue line in Fig. 9). In contrast, the method proposed here with a bit of adaptations can elegantly eliminate the peak interference. First recall that the Fourier coefficients of any noise are zero-mean circular complex Gaussian [62]. Consequently, the power spectral density of the noise, which is the squared modulus of the coefficients, obeys a chi-squared distribution with 2 degrees of freedom. Its probability density function is in fact a negative exponent, which happens to be the same distribution as a speckle noise obeys [63]. Since the speckle noise is usually modeled as a multiplicative noise [64], it is analogous to conclude that the noise in the Schottky spectrum is also multiplicative.

Therefore, a logarithmic transform should first be applied to the spectrum so as to use the additive model in Eq. (1). The transformed spectrum of length $n = 1639$ is then embedded into a partial circulant matrix of $m = 290$ rows. This time only the first two components are taken to reconstruct the background. As can be seen in Fig. 9, the resultant approximation of red line is in excellent agreement with the reference of green line, which is obtained by fitting a “bald” spectrum when particles are purged from the storage ring.

The proposed method hence opens up a possibility to deduct the resonant background *in situ*. It will be no longer necessary to interrupt an ongoing experiment just for the

FIG. 10. Weak peak detection in a Schottky spectrum by the proposed method in this work. (a) The red line is the denoised spectrum, and the green line, which is obtained by averaging 100 similar spectra, provides a reference. All local maxima in the red spectrum are marked with blue crosses, which also respectively indicate their prominences (vertical extent) and widths (horizontal extent). The detected peaks are labeled, in a descending order of PWR, as 1, 2, and 3. (b) The PWR of all eight peak candidates, among which the largest three are considered as real peaks associated with particles.

reference measurements, which increases effective on-target beam time. This is in particular useful in case the yields of aimed particles are extremely low.

C. Peak detection

Another common challenge in Schottky mass spectrometry is the detection of weak peaks. Figure 10(a) shows an example of such a case. Apart from the predominant peak in the center, it is impossible to unambiguously detect other peaks in the noisy spectrum. A normal solution is to continuously collect a number of spectra and average them to improve the SNR. For example, the green line in Fig. 10(a) is obtained from 100-fold averaging, which can barely reveal two weaker peaks on the left side. An obvious drawback of this approach is the degradation of time resolution, which, in this case, is 100 times worse. It is thus unfavorable for the time-resolved Schottky mass spectrometry [65], and in particular for the single-particle decay spectroscopy [66]. Even worse is that sometimes it is unfeasible to collect sufficient spectra, because, e.g., the aimed particle may have already decayed [67].

By using the proposed method, the noisy spectrum of length $n = 1639$ is first log-transformed and then embedded into a partial circulant matrix of $m = 430$ rows. A smoothed spectrum is reconstructed from the first seven SVD components, which is shown as the red line in Fig. 10(a). Peaks are searched among local maxima in the smoothed spectrum as the candidates. For each candidate, its prominence and width are subsequently measured, where the prominence is

the relative height from the summit to the highest adjacent valley, and the width is the horizontal span at half prominence [see blue crosses in Fig. 10(a) for illustration]. Afterwards, the prominence-to-width ratio (PWR), shown in Fig. 10(b), is calculated for each candidate to characterize its significance. Based on this parameter, in total three peaks are decisively identified with the largest PWRs and labeled with 1, 2, and 3 in Fig. 10(a). The remaining candidates are only considered as bumps due to their insignificant PWRs. It is clear in Fig. 10(a) that the detected peaks perfectly align with those in the averaged spectrum, and, moreover, with a 100-fold improvement of time resolving power.

Once the locations of weak peaks are coarsely determined from the smoothed spectrum, they can subsequently be transferred to a dedicated peak-finding algorithm as the required prior knowledge to refine the result [68]. What is more, the proposed method can be deployed to a real-time task to fast track particles in a dynamic process such as orbital-electron capture [69] or bound-state β^- decay [70] on an event-by-event basis.

V. CONCLUSION

An SVD-based one-dimensional data denoising scheme has been proposed. Owing to its nonparametric nature, it works for any additive noise, as well as multiplicative noise after logarithmic transform. By construction of a partial circulant matrix, the proposed method well balances computational simplicity and smoothing efficiency. The proposed NMTV criterion to select the optimal approximation rank allows for an integration into automated processes, which is a compelling feature for certain applications in reality. With the real-world data, the proposed method has proved its strong competitiveness among other nonparametric denoising methods such as moving average, wavelet shrinkage, and total variation. Furthermore, a few interesting applications of the method other than denoising were also addressed, and its competence has been demonstrated with cases in precision storage-ring mass spectrometry. Last, a Python implementation of the proposed method is provided and placed in the public domain [71].

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