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Properties of Savitzky–Golay digital differentiators

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Abstract

The Savitzky–Golay (SG) filters are generally used for smoothing and differentiation in many fields. The properties of the SG smoothing filters have been well studied. However, the properties of the SG differentiation filters or SG digital differentiators (SGDD, for the first order differentiation) are not developed well somehow, although they have been widely used. In the paper, the properties of the SGDD are discussed in detail. The effects of the SGDD on a noise-free single Gaussian line and a noise-free Gaussian doublet are studied via simulation. The results indicate that the contrast and resolution loss of the SGDD depends on the ratio of the width of signal derivative and filter length. The linear SGDD is not preferable for preserving small details of signal derivative from this study. The cubic and quintic SGDD with the choice of appropriate filter length are recommended in order to maintain the resolution of signal derivative.

Keywords: Savitzky–Golay; Digital differentiator; Differentiation; Property

1. Introduction

In various fields such as biomedical signal processing of electrocardiograph (ECG) and left ventricular pressure (LVP), numerical differentiation is important and necessary for extracting information about rapid transients contained in the signal [1–3]. In ultrasound

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elastography, a promising method for quantifying and imaging the elastic properties of biological tissues, the axial strain distribution within the tissues are calculated as the numerical differentiation of the estimated axial displacements [4,5]. Unfortunately, the numerical differentiation is an unstable and risky operation, and should be under taken with great caution because it can greatly amplify the noises, especially at high frequencies [1–3,6].

In the classical paper written by Savitzky and Golay [7], which has been cited more than 3800 times according to ISI Web of Science, a digital filter for smoothing and differentiation was developed to automatically perform the running least-squares polynomial fitting when the input signal was convolved with the filter coefficients. The numerous and typographic errors in the original tabular coefficients of the Savitzky–Golay (SG) smoothing and differentiation filter were subsequently corrected [8,9]. The closed-formed solutions have been derived by use of orthogonal polynomials (Gram polynomials or Legendre polynomials) [10–12] or a matrix approach [8,13]. In addition, the SG filter has been generalized for unequally (non-uniformly) spaced data [14], for initial or end points [11,15,16]. Commonly, the polynomial degree is fixed. However, the polynomial degree can vary according to the sum of squares of fitting residuals to obtain an adaptive-degree polynomial filter [17,18]. Similarly, the filter length may also be adaptively selected [19]. Furthermore, the SG filter has been extended to two-dimension [20–23], three-dimension [19], and multi-scale [24].

The SG filters have many advantages. Firstly, the intrinsic principle, i.e., the running least-squares polynomial fitting, is quite clear and straightforward. The convolution operation is much more easily implemented in algorithms than the least-squares calculation. Secondly, the filter coefficients can be easily obtained from a given table [7,8,11], from the explicit solution [9], or from some existing routines [25–28]. Moreover, the filter coefficients are all convenient integers except for an integer scaling factor, as may be especially significant in some applications such as those in some single-chip microcomputers or digital signal processors [3]. Thirdly, the SG filters can have arbitrary lengths (orders) and hence may be preferable in biological or biomechanical data processing (e.g., strain calculation in ultrasound elastography [4,5]) where the sampling frequency is usually low [3].

For a given order differentiation (zeroth differentiation = smoothing), the coefficients of the SG filters are dependent on the polynomial degree and the filter length [7–13]. To use the SG filters sophistically and select the polynomial degree and filter length appropriately, we must study their properties first. The properties of the SG smoothing filters have been well reviewed in Refs. [12,29–33]. However, as far as the authors know, the properties of the SG differentiation filters or the Savitzky–Golay digital differentiators (SGDD, for the first order differentiation, the same below) are not analyzed thoroughly in any published paper. Since the SGDD is frequently and widely used nowadays [5,34–39], the properties should be studied systematically in theory and in simulation. This is the motivation of this study. In this paper, we present a thorough analysis of the properties of the SGDD and make some suggestions for future applications. We do not focus on the significance of the SGDD or the calculation method of the filter coefficients (they are easily computed). What we focused on is the analysis of the SGDD properties, rather than the design of the filters like the window method [13,40,41], the frequency sampling method [13,40,41], the Parks–McClellan method [40,41] and some other methods [27].

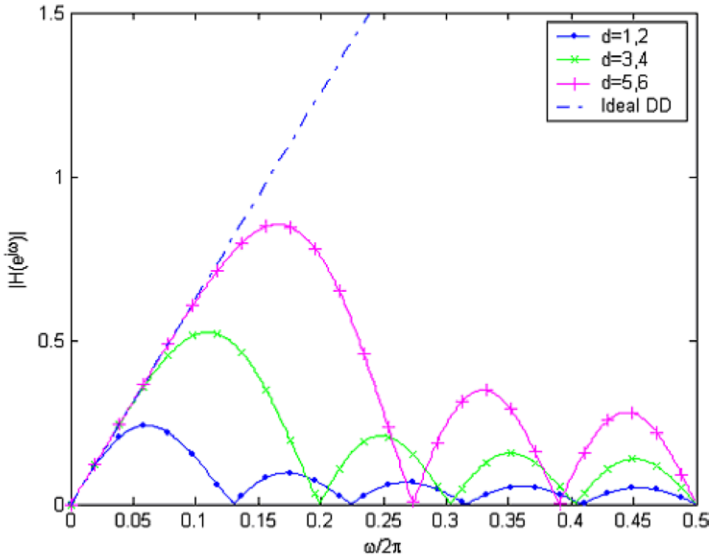


Fig. 1. Frequency responses of different degree SGDD ($2M + 1 = 11$).

2. Proprieties of SGDD in theory

2.1. Basic proprieties

Impulse responses of the SGDD are the same for central point differentiation with the use of either an odd polynomial degree or the next higher even degree, e.g., $1/2$, $3/4$, $5/6$, etc. [7–13]. In the paper, the SGDD of $d = 1/2$, $3/4$ and $5/6$ are referred to the linear, cubic and quintic SGDD, respectively. The impulse response of the SGDD is anti-symmetric [7–13]. Therefore, the SGDD belongs to the type III filter that has a linear phase [40].

Since the ideal digital differentiator (DD) greatly amplifies the noise, especially at high frequencies, one would be readily to choose a low-pass DD rather than a full-pass one [1–3,5,6]. According to the anti-symmetry, the frequency response of the SGDD is pure imaginary, which is quite close to the frequency response of the ideal DD ($H_{\text{ideal}}(e^{j\omega}) = j\omega$) at low frequencies. In addition, the frequency response of the SGDD is equal to zero at $\omega = \pi$. Therefore, the SGDD can be considered as a low-pass DD. Figure 1 shows the frequency responses (magnitude) of the linear SGDD, the cubic SGDD and the quintic SGDD at a length of $2M + 1 = 11$, as well as that of the ideal DD. As shown, the responses of the SGDD are close to that of the ideal DD at low frequencies, and attenuate much at high frequencies.

2.2. Impulse response restriction

As illustrated in Appendix A, the impulse response of the SGDD with a length of $2M + 1$ ($2M \geqslant d$) has the constraints written as

$$\sum_{n=-M}^{M} n^i h(n) = -\delta(i-1), \quad i = 0, 1, \ldots, d. \tag{1}$$

In the paper the constraint equations from $i = 0$ to d are derived.

2.3. *Frequency response flatness at $\omega = 0$*

When the constraints of the impulse response given above are used in the frequency domain the flatness constraints of the frequency response at $\omega = 0$ are obtained as (see Appendix B)

$$H^{(i)}(e^{j\omega})|_{\omega=0} = H^{(i)}_{\mathrm{ideal}}(e^{j\omega})|_{\omega=0} = j\delta(i-1), \quad i = 0, 1, \ldots, d. \tag{2}$$

As can been seen from Fig. 1, the frequency response of the SGDD is more flattened and is closer to the ideal DD at low frequencies as the polynomial degree d increases. However, the increase of the flatness is at the expense of a relatively higher cut-off frequency or a wider low-pass range. When $d = 2M$, the polynomial fitting is degenerated to the Lagrange interpolation, whose closed-form solution is given by [42]. According to the frequency response flatness at $\omega = 0$, it is the maximum flat DD [43], as has been proved in [42].

2.4. *Moments preservation of derivative of input signal*

Equivalent to the impulse response restriction, a dth degree SGDD exactly preserves the moments of the derivative of the input signal up to the order d. This can be derived as (see Appendix B)

$$\sum_{n} n^i y(n) = \sum_{n} n^i y_{\mathrm{ideal}}(n), \quad i = 0, 1, \ldots, d, \tag{3}$$

where $y(n)$ and $y_{\mathrm{ideal}}(n)$ are the output of the SGDD and the ideal derivative of input signal, respectively.

2.5. *Optimal filter to reduce noise amplification factor*

Assuming that the input signal is contaminated by independent Gaussian white noise (or a weaker condition of uncorrelated and homoscedastic noise), the noise amplification factor of a digital filter is given by the sum of the squares of the filter impulse response [6,13]. The noise amplification factors of various SGDD as a function of the filter length are given in Fig. 2. As the filter length increases or the degree of fitting polynomial decreases, the noise amplification factor deceases.

In statistics, the Gauss–Markov theorem states that the best linear unbiased estimators of the coefficients for a linear model with independent Gaussian white noise or errors (or a weaker condition mentioned previously) are the least-squares estimators [44], which are equivalent to the SGDD. In practice, if the input signal can be modeled by a polynomial added with Gaussian white noises, the SGDD can achieve the Cramer–Rao lower bound (CRLB) of estimation of signal derivative [45]. On the other hand, the constraints of $h(n)$

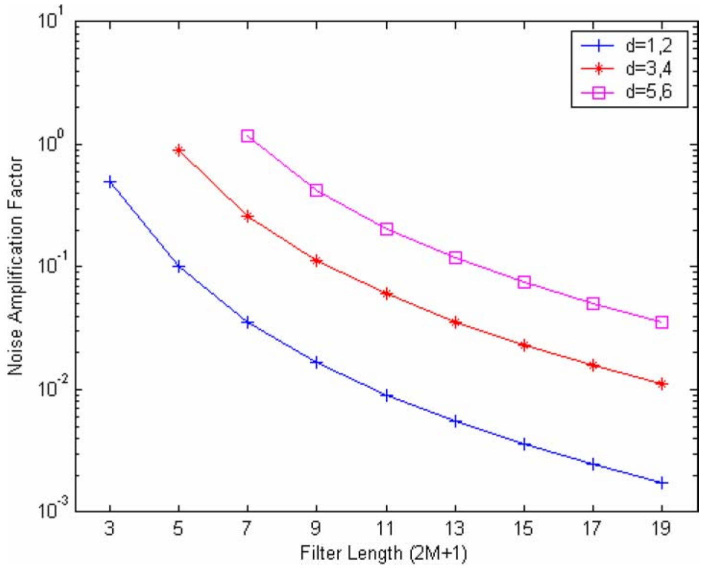


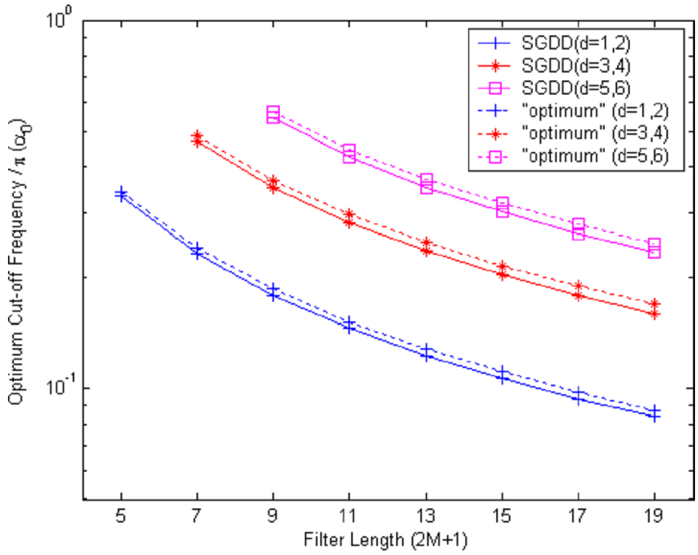
Fig. 2. Noise amplification factors of various SGDD.

given by Eq. (1) are necessary for an unbiased estimator of the derivative in a polynomial model with zero-mean noises. Therefore, the SGDD is an optimal DD in the sense of minimizing the noise amplification factor, but its impulse response is subject to additional constrains given by Eq. (1).

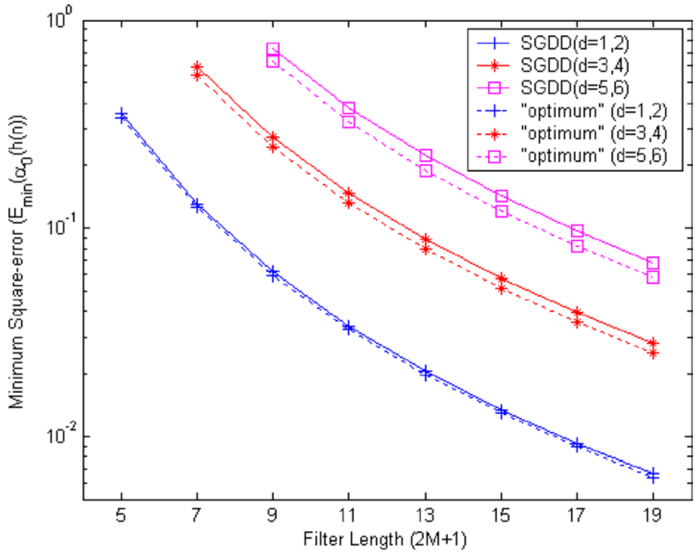
2.6. Optimum cut-off frequency and minimum square-error

In this paper, a specific measurement is presented to evaluate a low-pass DD and its functions. The specific measurement is the minimum square-error. This is because the minimum square-error can measure not only the "closeness" between the practical DD and the ideal DD at low frequencies, but also the noise elimination at high frequencies [3]. The optimum value of the cut-off frequency can be obtained by minimizing the square error of a given DD [3]. The optimum cut-off frequency of a DD represents its low-pass range to a certain extent. The square-errors can be further minimized to obtain the "optimum" DD by changing the impulse response of the DD under the constraint of anti-symmetry and those given by Eq. (1) [3].

Figure 3a shows the optimum cut-off frequencies and the minimum square-errors for the SGDD and Fig. 3b shows the optimum cut-off frequencies and the minimum square-errors for the "optimum" DD with length varying from 3 to 19. As the filter length increases or the fitting polynomial degree decreases, both the optimum cut-off frequency and the minimum square-error decrease. As shown, the minimum square-errors of the SGDD are very close to the minimum square-errors of the "optimum" DD, which represent the theoretical minimums under the certain constraints. Therefore the SGDD is almost the "optimum" DD in the sense of minimum square-error. Furthermore, their integer coefficients are more efficient than the floating-point of the "optimum" DD.



(a)

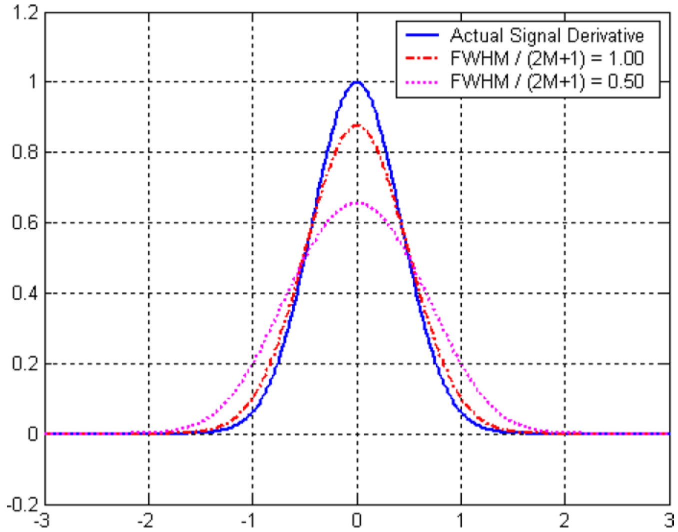


(b)

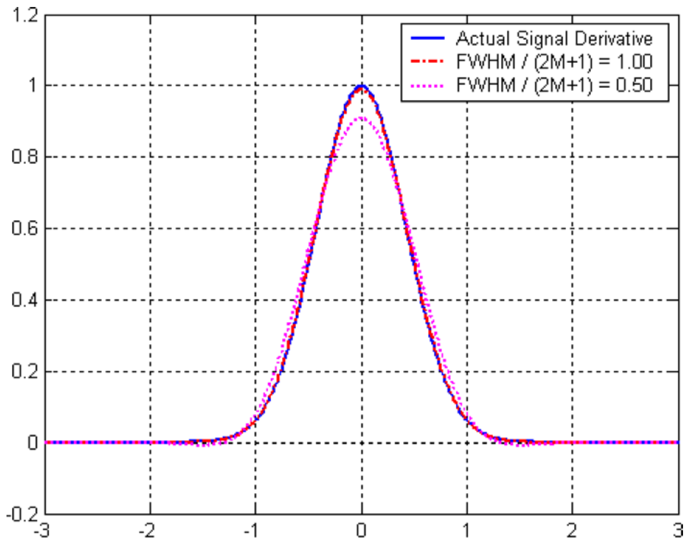
Fig. 3. Optimum cut-off frequencies (a) and minimum square-errors (b) of various SGDD and "optimum" DD.

3. Properties of SGDD in simulation

The analysis on the noise amplification factor and the optimum cut-off frequency may help select the appropriate SGDD to reduce the noise amplification, and to reject noise frequencies higher than the cut-off frequency at the same time.



(a)



(b)

Fig. 4. Effects of linear SGDD (a) and cubic SGDD (b) on a noise-free single Gaussian line.

It is expected that a higher polynomial degree or longer SGDD is more effective in removing noise, but at the expense of distorting small details (e.g., the contrast and resolution) of the signal derivative too much. In practice, the trade-off between noise reduction and contrast/resolution loss is inevitable with the use of the SGDD.

The contrast and resolution loss of the SG smoothing filters has been studied by evaluating the effects on a noise-free single Gaussian line and a noise-free Gaussian doublet [32,33]. A similar study on the SGDD are carried out in our work. The most important

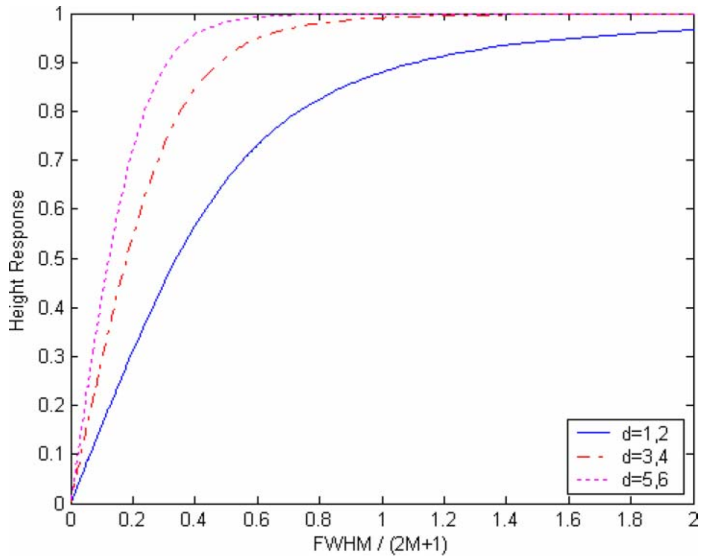


Fig. 5. Height response of SGDD on a noise-free single Gaussian line as a function of ratio of FWHM to filter length.

thing for the SGDD is the effect on the signal derivative rather than that on the input signal itself. Therefore in this paper, the underlying function of the signal derivative is assumed as a single Gaussian line or a Gaussian doublet, respectively. The input signal can be obtained explicitly by integrating the assumed function. The effects of the SGDD can be studied by comparing the output signal of the SGDD to the actual signal derivative. It is expected that the most important parameter in studying the effects is the ratio of the full width at half maximum (FWHM) of the signal derivative and the filter length [34], which is similar to the study of the SG smoothing filters [32,33]. It has been suggested that at least 10 points per FWHM are required to represent the Gaussian function without reconstruction [33]. In this study, the sampling interval is set to be $1/50$ FWHM, i.e., 50 data points per FWHM of the Gaussian function.

3.1. Contrast effects on a single line

Figure 4 illustrates the effects of the linear and cubic SGDD on a noise-free single Gaussian line, respectively. As the filter length increases, the height of the line decreases, and the width increases. It can be seen that a higher degree SGDD preserves the contrast of signal derivative better.

The height responses of the linear SGDD, cubic SGDD and quintic SGDD are shown in Fig. 5. The height response is defined as the ratio of the maximum value of the output signal after differentiation filtering to the actual maximum value of the signal derivative. As shown in Fig. 5, the height response of the linear SGDD is much lower than those of the cubic SGDD and quintic SGDD. For each kind of SGDD, the height response decreases as the filter length increases. The decrease of the height response may be related to the loss of contrast after passing the SGDD. The change of the sampling interval and the value of

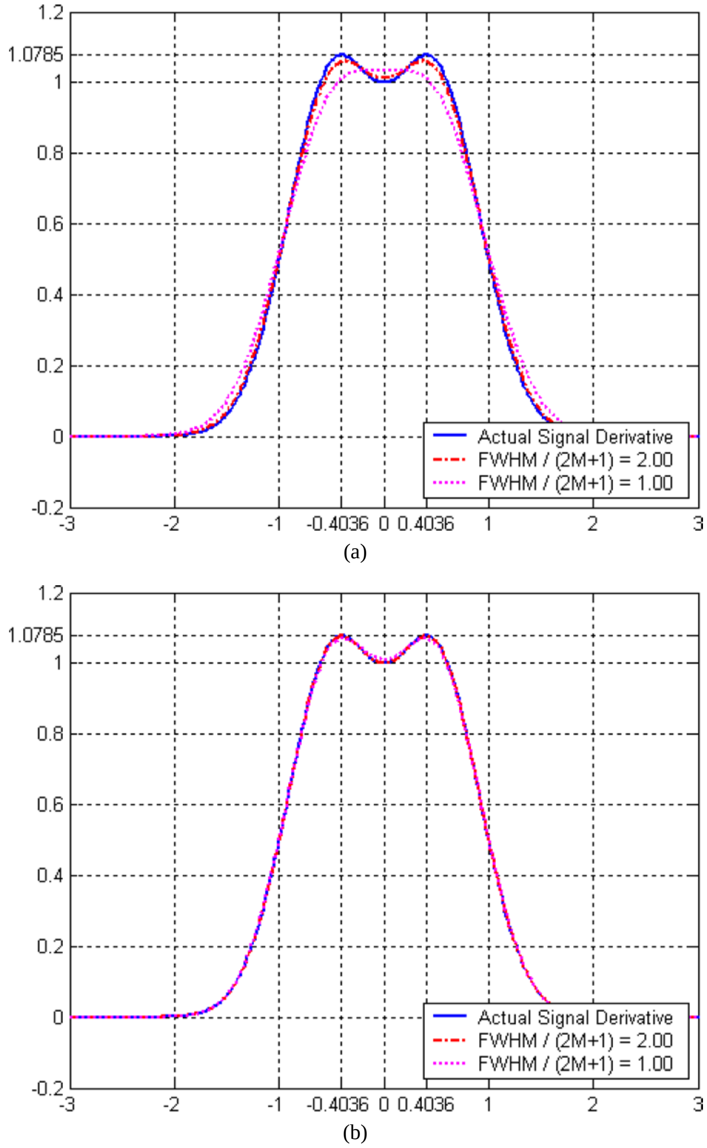


Fig. 6. Effects of linear SGDD (a) and cubic SGDD (b) on Gaussian lines with original dip of 7.85%.

FWHM can cause almost the same height response as a function of ratio of FWHM to filter length. Thus the height response is independent on the sampling frequency and FWHM.

3.2. Resolution effects on a doublet

To evaluate the resolution loss, a doublet model is used to check if two identical noise-free Gaussian functions can be resolved when their center distance is equal to the FWHM.

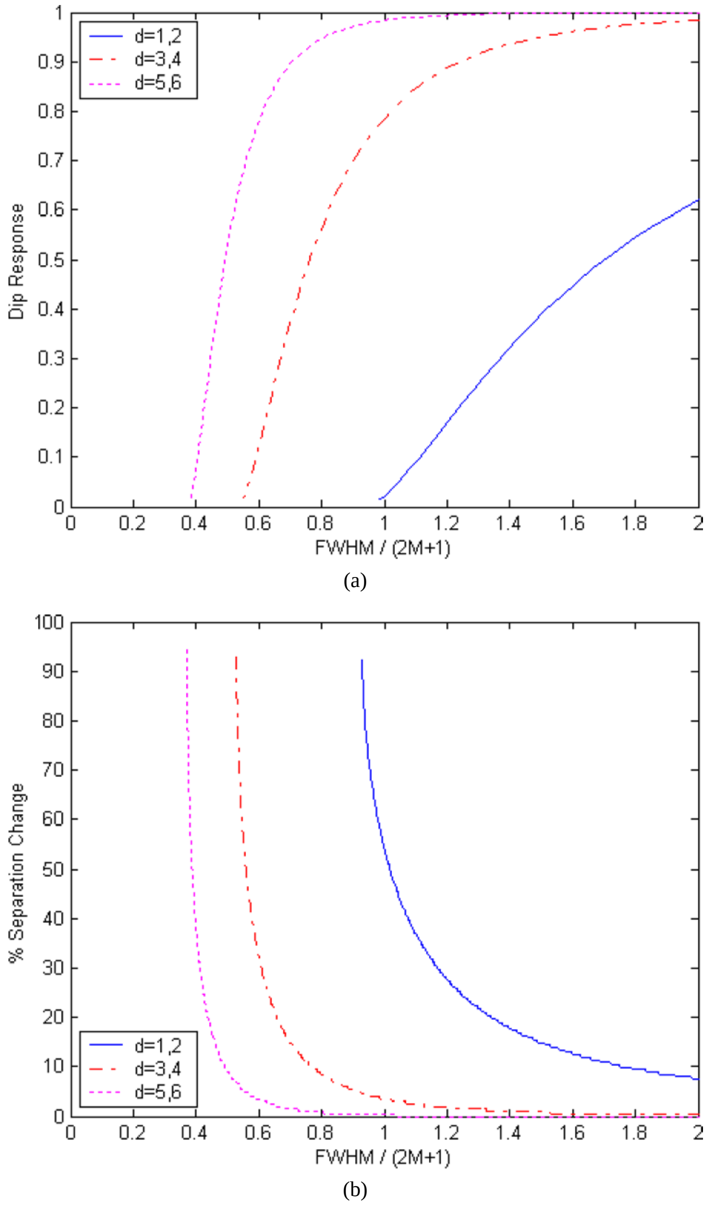


Fig. 7. Effects of SGDD on dip (a) and separation (b) of doublets having original dip of 7.85% as a function of ratio of FWHM to filter length.

Figure 6 shows the effects of the linear SGDD and cubic SGDD on a noise-free Gaussian doublet. The doublet had a 7.85% dip and a 0.8072 FWHM separation in this example. As the filter length increases, both the doublet percent dip and the peak separation decrease. The higher degree polynomial fitting can better preserve the resolution of the signal derivative. In particular, when a linear SGDD with $\mathrm{FWHM}/2M + 1 = 1.00$ is used, the doublet dip and the apparent peak separation are significantly distorted, as can be seen in Fig. 6a.

Figure 7a plots the dip response and Fig. 7b gives the change in peak separation as a function of the FWHM divided by the filter length. The dip response is defined as the ratio of the doublet percent dip after differentiation filtering to the original dip (i.e., 7.85%). As shown in these figures, the linear SGDD performs poorly with a much lower dip response, and a much higher change in peak separation. Therefore, the linear SGDD is not recommended to be used in terms of preserving the resolution of signal derivative, at least when the signal derivative is approximately modeled by a Gaussian doublet. A cubic SGDD with an optimal filter length of $\mathrm{FWHM}/(2M + 1) \geqslant 1.5$ and a quintic SGDD with $\mathrm{FWHM}/(2M + 1) \geqslant 0.8$ are recommended when the resolution is highly considered.

4. Discussion

As illustrated in Appendix C, a differentiation filtering on the signal can be regarded as a smoothing filtering on the derivative of the signal. According to the calculation [3], the optimum cut-off frequency of the differentiation filter is equal to the cut-off frequency of the decomposed smoothing filter at $1/2$ attenuation (-6 dB). Furthermore, the flatness constraints on the frequency response of the dth degree SGDD are equivalent to the flatness constraints on the frequency response of the smoothing filter $(H_1(e^{j\omega}))$, as shown in the following:

$$H_1^{(i)}(e^{j\omega})|_{\omega=0} = \delta(i), \quad i = 0, 1, \ldots, d - 1. \tag{4}$$

The cubic SGDD ($d = 3, 4$) satisfies the flatness of $H(e^{j\omega})$ at $\omega = 0$ up to the order 4, and the flatness of $H_1(e^{j\omega})$ at $\omega = 0$ up to the order 3. The quadratic SG smoothing filter ($d = 2, 3$) satisfies the flatness of $H(e^{j\omega})$ at $\omega = 0$ up to the order 3 [12,13,31–33]. Therefore the cubic SGDD applied to the signal is similar to the quadratic SG smoothing filter applied to the derivative of the input signal. The effects of the cubic SGDD on a noise-free single Gaussian line and a noise-free Gaussian doublet, such as the height response, the dip response and the separation change, are similar to the previous results of the quadratic SG smoothing filter [32,33].

5. Conclusion

In the paper, the properties of the SGDD are discussed in detail. Based on the thorough studies, it has been found that the dth degree SGDD exactly preserves the moments of the derivative of the input signal up to the order d. The SGDD minimizes the noise amplification factor with the impulse response restriction and moments preservation mentioned previously. In addition, the SGDD satisfies the flatness constraints on the frequency response at $\omega = 0$, and approaches the ideal DD at low frequencies. As the fitting polynomial degree decreases or the filter length increases, the noise variance is reduced, however, at the expense of eliminating some details of the signal derivative.

The simulation study can help understand the loss of contrast and resolution of the SGDD. The results indicate that the contrast and resolution loss of the SGDD depends on the ratio of the width of the signal derivative and the filter length. From this study, the cubic SGDD with a filter length satisfying $\mathrm{FWHM}/(2M+1) \geqslant 1.5$ and the quintic SGDD with $\mathrm{FWHM}/(2M+1) \geqslant 0.8$ are recommended. The linear SGDG is not recommended when the contrast and resolution is of consideration, because it cannot preserve the contrast and resolution of the signal derivative appropriately.

Acknowledgment

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Appendix A. Impulse response restriction

The matrix **G** that is related to the filter coefficients of the differentiation filter with different orders at the midpoint is given by [13]

$$\mathbf{G} = \mathbf{S}(\mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1} = [\mathbf{g}_0, \mathbf{g}_1, \ldots, \mathbf{g}_d], \tag{A.1}$$

where **S** is the basic matrix. Details can be found in [13].

From Eq. (A.1), we can derive

$$\mathbf{S}^{\mathrm{T}}\mathbf{G} = \mathbf{I}. \tag{A.2}$$

Expanding the second column of the left-hand of this equation and that of the right-hand side, respectively, Eq. (A.2) becomes

$$\sum_{n=-M}^{M} n^i g_1(n) = \delta(i-1), \quad i = 0, 1, \ldots, d, \tag{A.3}$$

where $\delta(n)$ is the discrete Dirac delta function.

Using the impulse response of the differentiation filter (the first order, the same below) $h(n)$ to replace the flip of $g_1(n)$, Eq. (A.3) becomes

$$\sum_{n=-M}^{M} n^i h(n) = -\delta(i-1), \quad i = 0, 1, \ldots, d. \tag{A.4}$$

The quantity in the left-hand side of Eq. (A.4) is called the ith moment of the impulse response which is related to the derivative of the frequency response at $\omega = 0$, by [13]

$$j^i H^{(i)}(e^{j\omega})|_{\omega=0} = \sum_n n^i h(n). \tag{A.5}$$

Comparing Eqs. (A.4) and (A.5), we obtain

$$H^{(i)}(e^{j\omega})|_{\omega=0} = j\delta(i-1), \quad i = 0, 1, \ldots, d. \tag{A.6}$$

Appendix B. Moments preservation of derivative of input signal

The frequency response $Y(e^{j\omega})$ of the output signal after passing a digital filter is given by

$$Y(e^{j\omega}) = X(e^{j\omega})H(e^{j\omega}), \tag{B.1}$$

where $X(e^{j\omega})$ and $H(e^{j\omega})$ are the frequency responses of the input signal and the digital filter, respectively. Differentiating Eq. (B.1) i times with respect to ω and using the product rules of differentiation, we obtain [13]

$$Y^{(i)}(e^{j\omega}) = \sum_{k=0}^{i} \binom{i}{k} H^{(k)}(e^{j\omega})X^{(i-k)}(e^{j\omega}). \tag{B.2}$$

Substituting the frequency response of the ideal DD ($H_{\text{ideal}}(e^{j\omega}) = j\omega$) into Eq. (B.2) and setting $\omega = 0$, Eq. (B.2) becomes

$$Y_{\text{ideal}}^{(i)}(e^{j\omega})|_{\omega=0} = jiX^{(i-1)}(e^{j\omega})|_{\omega=0}. \tag{B.3}$$

Similarly, substituting the frequency response constraints of the SGDD Eq. (A.6) into Eq. (B.2), we obtain

$$Y^{(i)}(e^{j\omega})|_{\omega=0} = jiX^{(i-1)}(e^{j\omega})|_{\omega=0}, \quad i = 0, 1, \ldots, d. \tag{B.4}$$

Comparing Eqs. (B.3) and (B.4) we obtain

$$Y^{(i)}(e^{j\omega})|_{\omega=0} = Y_{\text{ideal}}^{(i)}(e^{j\omega})|_{\omega=0}, \quad i = 0, 1, \ldots, d. \tag{B.5}$$

According to the relationship of the moments to the frequency response given by Eq. (A.5), we derive

$$\sum_n n^i y(n) = \sum_n n^i y_{\text{ideal}}(n), \quad i = 0, 1, \ldots, d, \tag{B.6}$$

where $y(n)$ and $y_{\text{ideal}}(n)$ are the output of the SGDD and the ideal derivative of the input signal, respectively.

Appendix C. Frequency response decomposition

The frequency response of a low-pass DD is given by

$$H(e^{j\omega}) = \frac{H(e^{j\omega})}{j\omega} j\omega = H_1(e^{j\omega})H_{\text{ideal}}(e^{j\omega}), \tag{C.1}$$

where $H_1(e^{j\omega}) = H(e^{j\omega})/j\omega$ can be regarded as the response of a low-pass filter or a smoothing filter, $H_{\text{ideal}}(e^{j\omega}) = j\omega$ represents the response of the ideal DD. Therefore the low-pass DD can be regarded to be constructed by cascading a smoothing (low-pass) filter with the ideal DD.

Assuming the frequency response of the input signal is given by $X(e^{j\omega})$, the frequency response of the output signal after passing the DD would be given by

$$Y(e^{j\omega}) = X(e^{j\omega})H(e^{j\omega}) = \left[X(e^{j\omega})j\omega\right]\frac{H(e^{j\omega})}{j\omega} = Y_{\text{ideal}}(e^{j\omega})H_1(e^{j\omega}), \tag{C.2}$$

where $Y_{\text{ideal}}(e^{j\omega}) = X(e^{j\omega})j\omega$ is the frequency response of the ideal derivate of the input signal. Therefore, the low-pass differentiation filtering on the input signal can be regarded as the smoothing filtering on the derivative of the input signal.

In addition, based on $H(e^{j\omega}) = H_1(e^{j\omega})j\omega$ we obtain

$$H^{(i)}(e^{j\omega})|_{\omega=0} = jiH_1^{(i-1)}(e^{j\omega})|_{\omega=0}. \tag{C.3}$$

Therefore, the flatness constraints up to the order d on the frequency response at $\omega = 0$ of the dth degree SGDD are equivalent to the flatness constraints up to the order $d - 1$ on the frequency response of the decomposed smoothing filter.

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