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Application Hints for Savitzky–Golay Digital Smoothing Filters

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The processing of spectra is often complicated by the presence of noise. The application of digital smoothing filters is a possibility for improving the accuracy of data extraction from those spectra. In this paper the fundamental properties of least-squares digital polynomial smoothing filters, popularized by Savitzky and Golay, are summarized. On the basis of these properties the range and the boundaries of application of these filters are discussed. They are seen to be approximately optimal in the range of low signal deformation.

Much has been written about least-squares digital polynomial smoothing filters (Savitzky–Golay smoothing filters in short), e.g. (*1–16*). They are probably the most frequently used digital smoothing filters in spectrometry. Nevertheless, there seems to be still some vagueness about their properties. Also, the question "In what cases are these filters superior over other types of digital smoothing filters?" has not yet been answered in a satisfactory manner. This paper lists some of the most significant properties of Savitzky–Golay smoothing filters in view of their appropriate applications.

Using the notation introduced in (*11*), a digital filter operator A is defined by

$$Af[k] = \sum_{n=-\infty}^{\infty} a[n]f[k-n] \qquad (1)$$

where f is the original spectrum with values $f[k]$, $k = 0, \pm 1, \pm 2, ...$, and a is the filter function. The brackets refer to the discrete character of the functions. For a Savitzky–Golay smoothing filter of degree $2M$ we may write

$$D_{2M}f[k] = \sum_{n=-N}^{N} a_{2M}[n]f[k-n] \qquad (2)$$

since $a_{2M}[n] = 0$ if $|n| > N$. The filter functions a_0, a_2, and a_4 will be found, e.g., in (*4, 11*). a_6 is derived with aid of the general formula given in (*18*)

$$a_6[n] = \beta(\alpha_0 + \alpha_2 n^2 + \alpha_4 n^4 + \alpha_6 n^6) \qquad (3)$$

where $\alpha_0 = 35N^6 + 105N^5 - 280N^4 - 735N^3 + 497N^2 + 882N - 180$, $\alpha_2 = -(315N^4 + 630N^3 - 1890N^2 - 2205N + 2121)$, $\alpha_4 = 693N^2 + 693N - 2310$, $\alpha_6 = -429$, and $\beta = 35/(4(2N-5)(2N-3)(2N-1)(2N+1)(2N+3)(2N+5)(2N+7))$.

PROPERTIES

The properties of Savitzky–Golay smoothing filters may be summarized as follows:

(1) Let p_{2M+1} be an arbitrary polynomial of degree $2M + 1$ or less, then

$$D_{2M}p_{2M+1} = p_{2M+1} \qquad (4)$$

That is, a Savitzky–Golay smoothing filter of degree $2M$ conserves every polynomial signal of degree up to $2M + 1$. Among all filters with filter width N ($2N + 1$ points) having this property, Savitzky–Golay smoothing filters perform maximal noise reduction for stationary white noise. Note that multiple filtering $D_{2M}{}^m$ also has the property (*4*)

$$D_{2M}{}^m p_{2M+1} = p_{2M+1} \qquad (5)$$

but does not show maximal noise reduction for a given filter width.

(2) If the moments μ_m of a signal f are defined by

$$\mu_m(f) = \sum_{k=-\infty}^{\infty} f[k]k^m \qquad (6)$$

it can be shown (*8*) that for every m with $0 \le m \le 2M + 1$

$$\mu_m(D_{2M}f) = \mu_m(f) \qquad (7)$$

That is, a Savitzky–Golay smoothing filter of degree $2M$ exactly conserves every existing moment up to $m = 2M + 1$. For practical requirements it may be sometimes reasonable to define "truncated" moments with the summation in eq 6 going over a finite interval $|k| \le K$ where K depends on the fwhm of the line. The effect of smoothing on area which is defined in such a way ("$\pm 2\sigma$ area") has been studied by Tominaga et al. (*12*). Enke and Niemann (*6*) empirically stated an increase in area ($\hat{\mu}_0(Df) > \hat{\mu}_0(f)$). The property of polynomial conservation (eq 4) appears to be completely equivalent to the conservation of moments (eq 7). So a Savitzky–Golay smoothing filter for a fixed width N is the moment conserving filter with most noise reduction. Note that for eq 7 to hold it is necessary and sufficient that the sum of all coefficients $a_{2M}[n]$ is one and all higher moments up to $m = 2M + 1$ are zero

$$\mu_0(a_{2M}) = 1 \qquad \mu_m(a_{2M}) = 0 \qquad (8)$$

The $(2M + 2)$th moment of the filter function a_{2M} is seen to be (*8*)

$$\mu_{2M+2}(a_{2M}) = \frac{(-1)^M 2((2M+1)!)^3}{(4M+3)!M!M!} \prod_{m=-M}^{M+1} (N+m) \qquad (9)$$

or, if N is large enough

$$\mu_{2M+2}(a_{2M}) \approx \frac{(-1)^M 2((2M+1)!)^3}{(4M+3)!M!M!} N^{2M+2} \qquad (10)$$

The $(2M + 2)$th moment allows an approximate calculation of the systematic error caused by smoothing, for further details see (*15*).

(3) Another description of digital filtering is obtained by Fourier transform (*3, 13, 14*)

$$\tilde{f}(\omega) = \sum_{n=-\infty}^{\infty} f[n] \exp(-i\omega n) \qquad |\omega| \le \pi \qquad (11)$$

realizing that filtering in frequency domain is equivalent to pointwise multiplication of the "frequency response" $\tilde{a}$ with the Fourier transform $\tilde{f}$ of the signal

$$(Af)^{\sim}(\omega) = \tilde{a}(\omega)\tilde{f}(\omega) \qquad (12)$$

Since the moments of the filter function are simply related to the frequency response and its derivatives at $\omega = 0$, eq 8 are equivalent to

$$\tilde{a}_{2M}(0) = 1 \qquad \tilde{a}^{(m)}(0) = 0 \qquad (13)$$

where $\tilde{a}^{(m)}$ denotes the mth derivative of $\tilde{a}$. In Figure 1 the frequency responses for the filters D_0, D_2, D_4, and D_6 are plotted ($N = 10$). Obviously Savitzky–Golay smoothing filters have a low-pass characteristic with flat passband.

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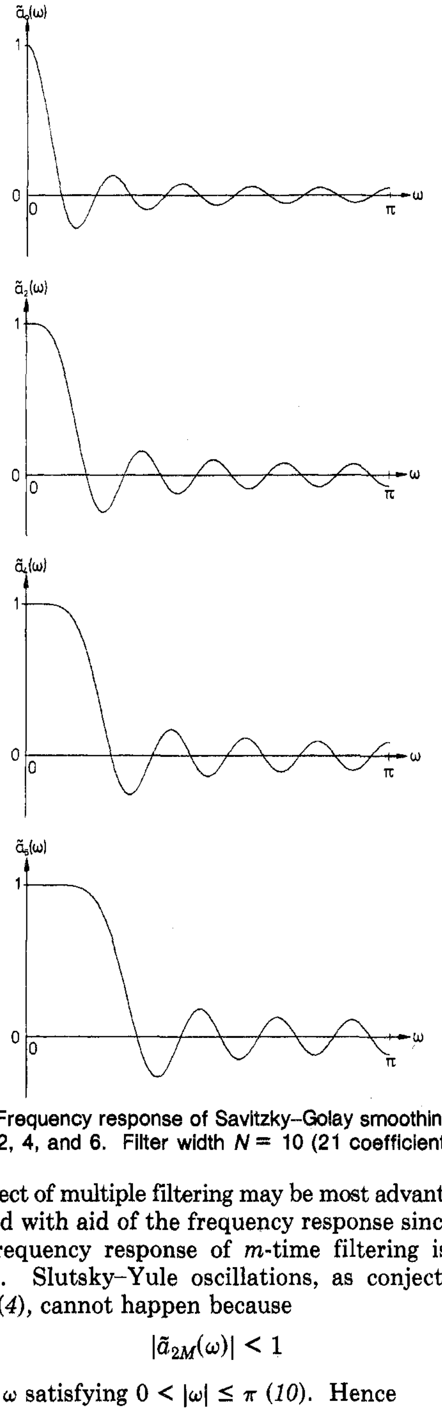

Figure 1. Frequency response of Savitzky–Golay smoothing filters of degree 0, 2, 4, and 6. Filter width N = 10 (21 coefficients).

The effect of multiple filtering may be most advantageously considered with aid of the frequency response since the resulting frequency response of m-time filtering is simply $(\tilde{a}_{2M}(\omega))^m$. Slutsky–Yule oscillations, as conjectured by Madden (*4*), cannot happen because

$$|\tilde{a}_{2M}(\omega)| < 1 \tag{14}$$

for every ω satisfying $0 < |\omega| \leq \pi$ (*10*). Hence

$$|\tilde{a}_{2M}(\omega)|^m \rightarrow 0 \tag{15}$$

if $m \rightarrow \infty$. Multiple smoothing is preferred if an improved high-frequency rejection is needed, e.g., if the subsequent processing is sensitive especially to high-frequency noise components (*3*). To avoid the loss of data points at the beginning and end of a record, Proctor and Sherwood (*24*) recently have proposed a combination of least-squares fitting and least-squares smoothing which enables every number of repeats desired.

(4) The noise reduction (assuming stationary white noise) of a digital filter is generally given by the inverse square root of the sum of squares of the coefficients $a[n]$ (*19*). In the case of Savitzky–Golay smoothing filters this simply reduces to the inverse square root of the coefficient $a_{2M}[0]$ (*8*)

$$\text{noise reduction} = (a_{2M}[0])^{-1/2} \tag{16}$$

Theoretically this result is independent of the probability density function of the noise. The deviation for uniform distribution, empirically obtained by Enke and Niemann (*6*) may be due to averaging too few samples.

Table I. Maximum Normalized S/N Enhancement for Some Smoothing Filters and Gaussian Peaks

filter	max normalized S/N enhancement	optimizing filter width (N resp RC) to fwhm ratio
matched	1	1
D_0	0.943	0.59
D_2	0.947	1.15
D_4	0.946	1.72
D_6	0.945	2.31
D_0^2	0.998	0.47
RC	0.895	0.88

RANGE OF APPLICATION

We have seen that a Savitzky–Golay smoothing filter acts as a low-pass that is optimal for polynomial signals. But in spectrometry we generally have nonpolynomial signals such as Gaussian or Lorentzian lines. The question may arise if or in which cases Savitzky–Golay smoothing is superior over other filtering techniques. This question can be answered by consideration of the statements of the last section.

Evidently, polynomial filtering becomes approximately optimal, if the spectrometric signal becomes approximately polynomial. That is, within the filter span ($2N + 1$ points), the signal f can be replaced by the first terms of its Taylor expansion fairly well such that

$$D_{2M}f \approx D_{2M}p_{2M+1} = p_{2M+1} \approx f \tag{17}$$

In the case of Gaussian or Lorentzian lines, condition 17 is fulfilled if the filter width is essentially smaller than the full width at half-maximum (fwhm) of the line

$$N \ll \text{fwhm} \tag{18}$$

Using the frequency representation, where the Fourier transform of the filtered signal $(D_{2M}f)^{\sim}$ is the product of the frequency response $\tilde{a}_{2M}$ (Figure 1) and the Fourier transform of the original signal (eq 12), we see that the filtered signal hardly differs from the original one, if all the transformed signal $\tilde{f}$ is concentrated in the flat region of the frequency response near $\omega = 0$. In other words, condition 17 is fullfilled for slowly varying signals, in accordance with inequality 18. Furthermore, in this weak filtering region, we can observe a decrease of error with increasing degree $2M$ of the Savitzky–Golay smoothing filter, if $2M$ is not too large (the maximum of $2M$ increases with decreasing maximal allowable error). A suggested value for the relative error is 1% or less, only slightly dependent on error criterion. Systematic signal distortion errors of this size can advantageously be calculated by using the moment approximation given by De Blasi et al. (*15*) together with eq 9. For Gaussian and Lorentzian lines the distortion of peak maximum (which in these cases is the largest systematic error occurring along the line) for a chosen noise amplification or filter width and polynomial degree can readily be obtained from the error diagrams in (*16*). Obviously, an operation in this low-error region is only reasonable if the statistical error after filtering and the signal distortion by filtering are of similar size. This is illustrated in Figure 2 where a noise-contaminated Gaussian peak f, having approximately 17 samples per fwhm, and its smoothed version D_4f, N = 12, are shown. Here the N to fwhm ratio is equal to 0.7, thus being well below the S/N optimizing ratio given in Table I. Giannelli/Altamura (*20*) and Papoulis (*21*) have developed simple expressions for the total error after weak filtering, including signal deformation and noise. This total error can

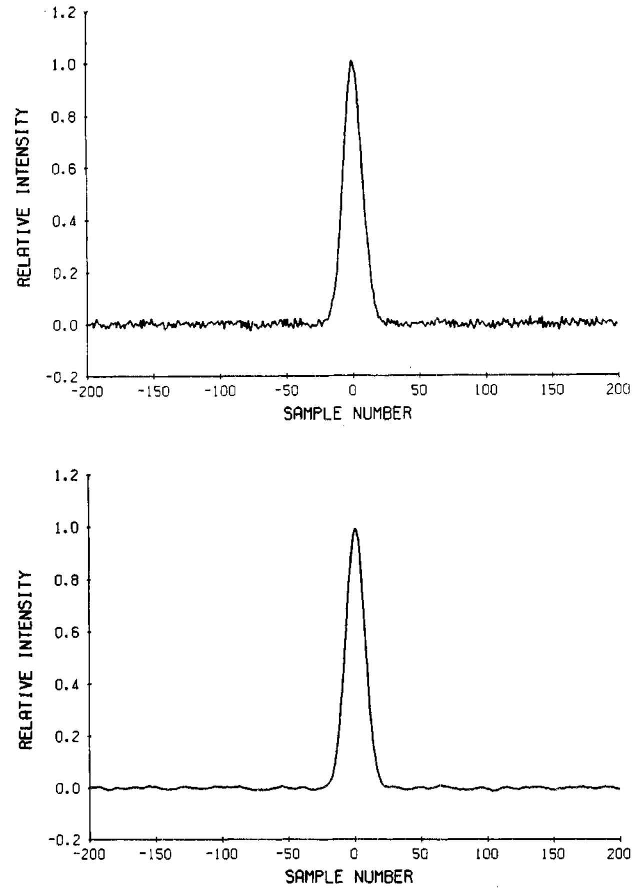

Figure 2. Unfiltered noisy Gaussian line and its weak filtered version. fwhm $\approx$ 17, filter degree $2M = 4$, filter width $N = 12$.

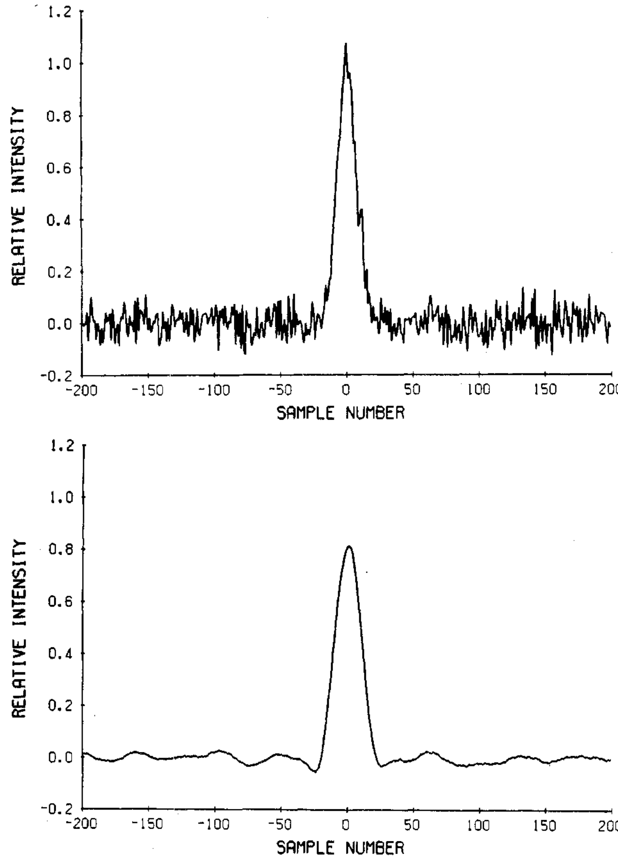

Figure 3. Unfiltered noisy Gaussian line and its S/N optimal filtered version. fwhm $\approx$ 17, filter degree $2M = 4$, filter width $N = 29$.

Table II. Maximum Normalized S/N Enhancement for Some Smoothing Filters and Lorentzian Peaks

filter	max normalized S/N enhancement	optimizing filter width (N resp RC) to fwhm ratio
matched	1	1
D_0	0.906	0.70
D_2	0.904	1.44
D_4	0.903	2.22
D_6	0.903	3.01
$D_0{}^2$	0.982	0.62
RC	0.899	1.12

be minimized with respect to the filter width (*20, 21*).

The case of weak filtering significantly differs from the case of maximizing signal to noise ratio (S/N). Here the filter width of a Savitzky–Golay smoothing filter of degree $2M$ is adjusted so that the S/N enhancement by filtering is maximized for a known shape and fwhm of the signal. The S/N ratio is defined by the peak height to standard deviation (σ) ratio. As is well-known, the absolute maximum S/N enhancement will be obtained with a matched filter. That is a filter whose filter function has the same shape and fwhm as the undistorted signal. Let the normalized S/N enhancement by a matched filter for a Gaussian line be 1. The corresponding approximate values for Savitzky–Golay smoothing filters and the RC filter are shown in Table I and Table II. The maximal achievable S/N-enhancement by Savitzky–Golay smoothing filters is seen to be only 5% smaller than the theoretical optimum.

Figure 3 shows the same line as Figure 2 except for increased noise. This time high-precision filtering is not suitable for the reason given above. So we have chosen $N = 29$ (N/fwhm ≈ 1.74) which is nearly the S/N optimizing filter width for D_4 and this line. It is an interesting fact that double filtering with D_0 achieves a higher maximum S/N enhancement than single pass filtering by arbitrary Savitzky–Golay smoothing filters. This arises from the theoretical result that the maximum of S/N enhancement directly depends on the likeness between the signal shape and the shape of filter function. The corresponding filter function of $D_0{}^2$ is a triangle and triangles give a better approximation of Gaussian peaks than any Savitzky–Golay smoothing filter functions. For higher degrees and higher iterates see Figure 5 of Proctor and Sherwood (*24*). Obviously, in the S/N maximizing case, it is true that Savitzky–Golay smoothing is not optimal, but the maximum achievable S/N enhancement only unessentially differs from the theoretical boundary.

At first sight it is not evident what degree $2M$ should be. In contrast to the case of weak filtering, where $2M = 2$ or 4 seems to be an appropriate choice, the authors recommend D_0 for S/N maximizing purposes since it is the simplest of all Savitzky–Golay smoothing filters, has the least optimal N, and does not produce any side lobes, which may lead to systematic faulty detections in automatic peak searching procedures. In Figure 4 an original undistorted Gaussian peak $f[k] = \exp(-k^2/100)$, fwhm ≈ 16.7, the optimal filtering D_4f with $N = 29$ (see Table I), and two filterings with mismatched N to fwhm ratio (broadest peaks, $N = 50$, N/fwhm ≈ 3 and $N = 100$, N/fwhm ≈ 6) are shown.

A third area of application for Savitzky–Golay smoothing filters may be background estimation or background subtraction for a slowly varying background b such that

$$\text{fwhm} \ll N \ll K \tag{19}$$

$$D_{2M}b \approx b \tag{20}$$

where K is the total number of measurements. If the filter width N is much greater than the maximal fwhm, occurring

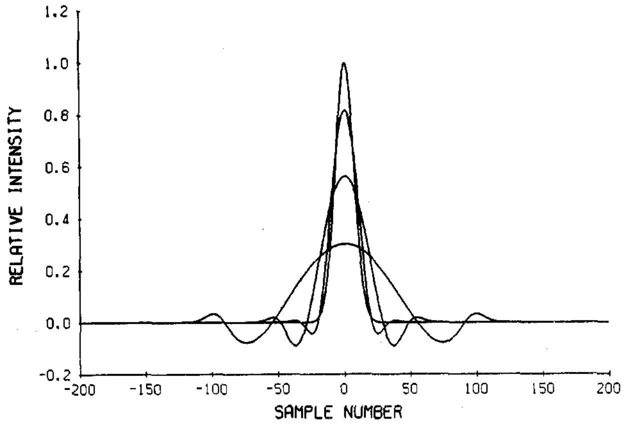

Figure 4. Deformation of a Gaussian line (high peak). Filter degree $2M = 4$. N/fwhm = 1.74, 3 (medium peaks), and 6 (low peak).

in the spectrogram, the peaks will be flattend (*22, 23*) and the background will remain for subtraction provided that the background can be approximated by a polynomial of degree $2M + 1$ within the filter width, and the number of peaks is relatively small. For "straightening through smoothing" applications the recursive representation of Savitzky–Golay smoothing filters (see ref 11) can most advantageously be used.

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Steady-State Theory of Biocatalytic Membrane Electrodes

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A mathematical derivation is presented for the exact solution of partial differential equations describing the steady-state response of biocatalytic potentiometric membrane electrodes. The derivation is based upon a previously proposed model in which the steady-state response is seen to result from a combination of diffusion and Michaelis–Menten kinetic steps. The expressions derived in this work yield further insight into the behavior of biocatalytic potentiometric membrane electrodes and permit convenient evaluation of key parameters as a function of the major experimental variables.

The empirical development of bioselective membrane electrodes (*1*) has proceeded rapidly in recent years with the recognition that bacterial cells, mitochondria, or intact animal and plant tissue slices can (*2*) be employed as biocatalysts at membrane electrode surfaces in a manner analogous to conventional enzyme electrodes. The concomitant development of theoretical models and formulations has not kept pace with these practical advances; recently, Brady and Carr (*3*) gave a theoretical treatment of the steady-state response of potentiometric enzyme electrodes but were limited to numerical evaluations of the resulting differential equation. We now develop an exact solution which can be more conveniently employed without the need for extensive computing facilities.

If we assume, as did Brady and Carr, that the net equation governing the rate of change of substrate concentration within any portion of the biocatalyst-containing membrane surrounding the sensor must contain a diffusional mass transport term and a Michaelis–Menten kinetic term, we obtain

$$\frac{\partial C_s}{\partial t} = D_s \frac{\partial^2 C_s}{\partial X^2} - \frac{k_2[\mathrm{E}_0]C_s}{K_M + C_s} \tag{1}$$

where D_s is the substrate diffusion coefficient in the membrane, C_s is the substrate concentration, $k_2[\mathrm{E}_0]$ is the biocatalyst activity, and K_M is the Michaelis–Menten constant. It is assumed that biocatalytic activity can be treated in a manner analogous to enzyme activity for the purposes of this model.

The schematic model of Brady and Carr is adapted to our notation in Figure 1 where the boundary condition is that $\partial C_s/\partial X = 0$ at $X = 0$ and $\partial C_s/\partial t = 0$ at steady state. Equation 1 then becomes

$$D_s \frac{\partial^2 C_s}{\partial X^2} - \frac{k_2[\mathrm{E}_0]C_s}{K_M + C_s} = 0 \tag{2}$$

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