An Optimal Weighting Function for the Savitzky-Golay Filter

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Abstract

The Savitzky-Golay FIR digital filter is based on a least-squares polynomial fit to a hypothetical sample of equally spaced data. This gives the filter the ability to preserve moments of features like peaks in the input. Descriptions of the filter typically consider the case where equal weights are implicitly applied to the residuals of the fit. In a largely overlooked paper Turton showed that weighting the residuals with a triangular function significantly improves the frequency response of the filter in the stopband. The Savitzky-Golay filter is commonly referred to as a smoothing filter. This paper uses a particular measure of smoothness to show that a quadratic residual weighting function optimizes the smoothness of the filter output for a given sample size and degree of the fitting polynomial. This weighting function can provide substantially better smoothness than that with a constant weighting function.

1 Introduction

In a 1964 paper Savitzky and Golay [1] showed how a least-squares polynomial fit to a sample of equally spaced data could be used as the basis of an FIR digital filter to smooth the noisy data typically generated by chemical analysis instruments like spectrometers. This paper has the distinction of being one of the most cited papers in the field of analytical chemistry. But as Schafer [2] has observed, the Savitzky-Golay (S-G) filter is not widely known within the digital signal processing community. This is partly because the frequency response of the S-G filter in the stopband region is mediocre. In a 1992 paper Turton [3] showed that weighting the least-squares residuals with a triangular function significantly improves the frequency response of the S-G filter in the stopband. However citation indices give relatively few citations for his paper which suggests that it merits more attention than it has received. This paper extends Turton’s analysis by showing that a quadratic weighting function optimizes a particular time-domain measure of the smoothness of the output of the S-G filter.

The material in this paper involves two disciplines, statistics and signal processing. The statistics term “measurement error” roughly corresponds to the signal processing term “noise”. For the purpose of this discussion it will be assumed that the measurement error or noise is an independent and identically distributed (i.i.d.) random variable with zero mean and that the true measurements or signal are smooth enough to be locally represented by a polynomial. Where this paper discusses statistical concepts and theory the terms “measurement” and “error” are used.
2 The Savitzky-Golay Smoothing Filter

This section shows how the Savitzky-Golay (S-G) filter is derived from the statistical theory of the optimal polynomial fit to a sample of measurements corrupted by random measurement error. It is assumed that \( q \) values of a hypothetical dependent variable, \( y \), are associated with \( q \) equally spaced values of an independent variable, \( x \), and that the relationship between \( x \) and \( y \) can be represented by a polynomial over the range of the \( q \) samples. To illustrate, if a quadratic equation in \( x \) with three unknown parameters, \( a_1, a_2, \) and \( a_3 \) is to be fit to five corresponding measurements of \( y \) then this can be expressed by the following set of five equations in three unknowns:

\[
\begin{align*}
y_1 &= a_1 + a_2 x_1 + a_3 x_1^2 \\
y_2 &= a_1 + a_2 x_2 + a_3 x_2^2 \\
y_3 &= a_1 + a_2 x_3 + a_3 x_3^2 \\
y_4 &= a_1 + a_2 x_4 + a_3 x_4^2 \\
y_5 &= a_1 + a_2 x_5 + a_3 x_5^2
\end{align*}
\] (2.1)

The number of unknown parameters, \( a \), will be denoted by \( n \). So in this case \( q = 5 \) and \( n = 3 \). Using matrix notation Equations 2.1 are more compactly expressed as:

\[
Xa = y
\] (2.2)

where \( X \) is a \( 5 \times 3 \) matrix the first column of which is a vector of ones, the second column is the vector \( x \) and the third column is the vector of the squares of \( x \). For the purpose of deriving a smoothing filter the scale of \( x \) doesn’t matter but it will be assumed that the values of \( x \) are equally spaced.

Because there are more equations for the elements of vector \( a \) than there are elements of \( a \) there won’t be a solution for \( a \) that exactly satisfies all of the equations if there is random error associated with the dependent variable, \( y \). The system of equations is said to be over-determined. The classic least-squares solution to a system of overdetermined linear equations gives values of the elements of the vector \( a \) that minimizes the sum of squares of the elements of the residual vector, \( \rho \), given by:

\[
\rho = Xa - y
\] (2.3)

This optimal values of the elements of vector \( a \) are obtained by premultiplying both sides of Equation 2.2 by the transpose, \( X^T \), of the matrix \( X \) which yields a matrix equation whose solution minimizes the sum of squares of the residuals which can be expressed as \( \rho^T \rho \):

\[
a = (X^TX)^{-1}X^Ty
\] (2.4)

The values of the polynomial fit are given by the vector \( \hat{y} \) which is the best estimate of the true values of the measurements:

\[
\hat{y} = Xa = X (X^TX)^{-1}X^Ty
\] (2.5)

If a particular element of the \( \hat{y} \) vector is of interest, say the \( j \)th element, then that element can be isolated from \( \hat{y} \) by a simple matrix operation. The vector \( u \) is constructed with \( q \) elements all of which are set to zero except for the \( j \)th element which is set to one:

\[
u_i = \begin{cases} 
0 & \text{for } i \neq j \\
1 & \text{for } i = j 
\end{cases} \quad \text{(for } i = 1 \ldots q) \] (2.6)

The \( j \)th element of \( \hat{y} \) is now given by:

\[
\hat{y}_j = u^T \hat{y} = u^T X (X^TX)^{-1}X^Ty
\] (2.7)
The transpose of \( u^T X (X^T X)^{-1} X^T \) is a vector of \( q \) filter coefficients, \( c \), which is independent of the elements of the vector \( y \):

\[
c = X (X^T X)^{-1} X^T u
\]  

(2.8)

Therefore the filtering operation is simply the dot product or convolution of the filter coefficients, \( c \), with the measurements, \( y \):

\[\hat{y}_j = c^T y\]  

(2.9)

The last two equations define the standard S-G smoothing filter. If the filter parameters, \( q \) and \( n \), are selected to avoid overfitting or underfitting the values of the filter input then features of the filter input that can be represented by the fitting polynomial will pass through the filter without distortion.

To summarize, the elements of the vector \( \hat{y} \), given by the polynomial fit, Equation 2.5, are the best estimates of the true values of the elements of the measurement vector \( y \). The \( j \)th element of the vector \( u \) in Equation 2.7 is set to one therefore \( u^T \hat{y} \) selects the \( j \)th element of \( \hat{y} \), the scalar \( \hat{y}_j \). Statistical estimation theory shows that the optimal value of \( j \) corresponds to the middle element of \( \hat{y} \) with index \((1+q)/2\) and for which \( u_{(1+q)/2} = 1 \). When \( j = (1+q)/2 \) then \( c \) is a symmetric vector and the filter is linear phase. In this case the value of \( q \) must be odd.

This standard description of the S-G filter implicitly assigns equal weights to the residuals, \( \rho \), in calculating the sum of squares of the residuals which can be expressed as \( \rho^T \rho \). A weighted sum of squares of the residuals can be expressed as \( \rho^T W \rho \) where \( W \) is a \( q \times q \) matrix of weights. In statistical estimation theory the optimal weight matrix \( W \) is the inverse of the error variance-covariance matrix. Because the measurement errors are assumed to be independent the weight matrix \( W \) can be taken to be diagonal. The value of the filter coefficient vector, \( c \), that minimizes the weighted sum of squares of the residuals, \( \rho^T W \rho \), is given by:

\[
c = WX (X^T WX)^{-1} X^T u
\]  

(2.10)

The derivative of the vector \( c \) with respect to the diagonal element \( W_{k,k} \) is given by:

\[
\frac{dc}{dW_{k,k}} = \left[ I - WX (X^T WX)^{-1} X^T \right] \frac{dW}{dW_{k,k}} X (X^T WX)^{-1} X^T u
\]  

(2.11)

where \( I \) is a \( q \times q \) identity matrix and \( dW/dW_{k,k} \) is a \( q \times q \) diagonal matrix with only one nonzero element which is one:

\[
\left[ \frac{dW}{dW_{k,k}} \right]_{i,i} = \begin{cases} 0 & \text{for } i \neq k \\ 1 & \text{for } i = k \end{cases} \quad \text{(for } i = 1 \ldots q)\]  

(2.12)
3 The Smoothness of the Output of an FIR Filter

The last section described the standard (i.e., equal residual weights) and the weighted version of the S-G smoothing filter. The smoothness of the output of a general FIR filter will now be quantified. If the impulse to the filter represents a unit input of measurement error (noise) then the filter distributes the unit impulse of error over an output response vector equal to the coefficient vector. This distribution of an unit input impulse of error over an output vector response can be described as a smoothing operation.

The output of a general FIR filter, $y$, is a convolution of the filter coefficients and the filter input:

$$y = c_1y_1 + c_2y_2 + \cdots + c_qy_q$$  \hspace{1cm} (3.1)

The values of the filter input, $y_i$, can be considered as having two additive components, the “true” values of the input and the errors. Because the filtering transformation is linear the filter’s action on the input errors can be analysed independently of the “true” values of the input. The error component of the filter input will be denoted by $e$ and the error component of the filter output, $e$, is given by:

$$e = c_1e_1 + c_2e_2 + \cdots + c_qe_q$$  \hspace{1cm} (3.2)

It is assumed that the values of the input error, $e_i$, are uncorrelated random variables with a mean of zero and constant variance, $\sigma^2_e$. With this assumption the variance of the output error, $\sigma^2_e$, is given by:

$$\sigma^2_e = c_1^2\sigma^2_e + c_2^2\sigma^2_e + \cdots + c_q^2\sigma^2_e$$  \hspace{1cm} (3.3)

The ratio of the variance of the filter output error to the variance of the input error, the error reduction ratio (aka noise reduction ratio), will be denoted by $r$ and is given by:

$$r = \frac{\sigma^2_e}{\sigma^2_e} = c_1^2 + c_2^2 + \cdots + c_q^2 = c^Tc$$  \hspace{1cm} (3.4)

The output error, $e$, can be considered to be smooth to the extent that the difference between successive values of the output error is small. The difference between successive values of the output error is:

$$\Delta e = (c_1e_2 + c_2e_3 + \cdots + c_qe_{q+1}) - (c_1e_1 + c_2e_2 + \cdots + c_qe_q)$$  \hspace{1cm} (3.5)

Rearranging terms and padding with zeroes gives:

$$\Delta e = (0 - c_1)e_1 + (c_1 - c_2)e_2 + \cdots + (c_{q-1} - c_q)e_q + (c_q - 0)e_{q+1}$$  \hspace{1cm} (3.6)

Padding with zeroes makes this equation symmetric with respect to all of the filter coefficients, particularly $c_1$ and $c_q$. The variance of the difference between successive values of the output error is:

$$\sigma^2_{\Delta e} = (0 - c_1)^2\sigma^2_e + (c_1 - c_2)^2\sigma^2_e + \cdots + (c_q - c_{q-1})^2\sigma^2_e + (c_q - 0)^2\sigma^2_e$$  \hspace{1cm} (3.7)

The ratio of the variance in the difference between successive values of the output error to the variance in the difference between successive values of the input error will be denoted by $s$ given by:

$$s = \frac{\sigma^2_{\Delta e}}{\sigma^2_{\Delta e}} = \frac{1}{2} \left[(0 - c_1)^2 + (c_1 - c_2)^2 + \cdots + (c_{q-1} - c_q)^2 + (c_q - 0)^2\right]$$  \hspace{1cm} (3.8)

This ratio, $s$, is a measure of the filter effectiveness in smoothing error (noise) and will be referred to here as the filter smoothing parameter. The factor of two is due to the fact that the variance in the difference between successive values of the input error is twice the variance of the input error.
Like the error reduction ratio of Equation 3.4, the smoothing parameter characterizes the filter itself and is independent of the filter input. In the degenerate case where $q = 1$ and $c_1 = 1$ the filter output is equal to the filter input and the values of both the error reduction ratio, $r$, and the smoothing parameter, $s$, are one. If $c$ were a stochastic variable then $s$ would be one minus the autocorrelation in $c$ or, equivalently, one minus the autocorrelation in the filter impulse response.

The padding with zeroes in Equation 3.8 serves to emphasize an important point. The output of an FIR filter will be smooth to the extent that the terms $(c_{i+1} - c_i)^2$ in this equation are small. When the residuals of the S-G filter are given equal weights then the terms $(0 - c_1)^2$ and $(c_q - 0)^2$ tend to dominate the other terms in value. It will be shown that an alternative residual weighting function will reduce the influence of these two terms on the filter smoothness.

Equation 3.8 can be expressed in compact matrix notation as:

$$s = \frac{c^T T c}{2}$$

where $T$ is a tridiagonal matrix whose elements are two on the diagonal and minus one on the off-diagonals:

$$T_{i,i} = 2 \quad \text{(for } i = 1 \ldots q)$$

$$T_{i,i+1} = T_{i+1,i} = -1 \quad \text{(for } i = 1 \ldots q - 1)$$

(3.10)

The derivative of the scalar $s$ with respect to the elements of vector $c$ is given by:

$$\frac{ds}{dc} = T c$$

(3.11)

### 4 The Optimal Weight Matrix For the Smoothing Parameter

The vector $v$ is constructed with $q$ elements all of which are one:

$$v_i = 1 \quad \text{(for } i = 1 \ldots q)$$

(4.1)

The weight vector $w$ is defined as:

$$w = T^{-1} v$$

(4.2)

where $T$ is given by Equation 3.10. The residual weight matrix, $W$, is diagonal and the elements of the diagonal correspond to the elements of the weight vector $w$:

$$W_{i,i} = w_i \quad \text{(for } i = 1 \ldots q)$$

(4.3)

It will now be shown that the smoothing parameter $s$ is minimized with respect to the elements of the weight vector $w$ defined by Equation 4.2. From Equations 4.1 and 4.3 it follows that:

$$W v = w$$

(4.4)

Premultiplying Equations 4.2 and 4.4 by $T$ gives:

$$T W v = v$$

(4.5)

Therefore $v$ is an eigenvector of $T W$ where the corresponding eigenvalue, $\lambda$, is one. The matrix $T W$ has $q$ eigenvalues given by:

$$\lambda_i = \frac{i(i+1)}{2} \quad \text{(for } i = 1 \ldots q)$$

(4.6)
If the first \( n \) eigenvectors are assembled columnwise into the \( q \times n \) matrix \( V \) then:

\[
TWV = VA
\]

(4.7)

where \( A \) is a diagonal matrix of the first \( n \) eigenvalues:

\[
A_{j,j} = \lambda_j \quad \text{for } j = 1 \ldots n
\]

(4.8)

Because the matrix \( TW \) is not symmetric the eigenvectors will not be orthogonal. However the eigenvectors are orthogonal with respect to the weight matrix \( W \). In other words the matrix \( V^TWV \) is diagonal. If the eigenvectors are scaled to be orthonormal with respect to \( W \) then the scaled eigenvectors, denoted by \( A \), are given by:

\[
A_{i,j} = \frac{V_{i,j}}{\sqrt{(V^TWV)_{j,j}}} \quad \text{for } i = 1 \ldots q, j = 1 \ldots n
\]

(4.9)

Therefore:

\[
A^TW = I
\]

(4.10)

and

\[
TW = AA
\]

(4.11)

Now, the columns of the matrix \( X \) in Equation 2.2 are a set of basis vectors based on increasing powers of the vector \( x \). With the eigenvalues given in the order of Equation 4.6 the first column of the matrix \( A \) is a constant, the second column is a linear function of \( x \), the third is quadratic, etc. Therefore the columns of the matrix \( A \) are an alternative set of basis vectors that have the property of being orthonormal. This means that wherever the matrix \( X \) appears in the equations of Section 2 it can be replaced by the matrix \( A \). With this substitution Equations 2.10 and 2.11 simplify to:

\[
c = WAA^Tu
\]

(4.12)

and

\[
\frac{dc}{dW_{k,k}} = \left[ I - WAA^T \right] \frac{dW}{dW_{k,k}} AA^Tu \quad \text{for } k = 1 \ldots q
\]

(4.13)

The derivative of the smoothing parameter \( s \) with respect to the element of the diagonal weight matrix \( W_{k,k} \) is obtained by combining Equations 3.11, 4.12 and 4.13:

\[
\frac{ds}{dW_{k,k}} = \left[ \frac{dc}{dW_{k,k}} \right]^T \frac{ds}{dc} = u^T AA^T \frac{dW}{dW_{k,k}} \left[ I - AA^T W \right] TWAA^T u
\]

(4.14)

To show that \( s \) is minimized with respect to the elements of the weight vector, \( w \), given by Equation 4.2 it is necessary to show that \( \frac{ds}{dW_{k,k}} \) is zero for \( k = 1 \ldots q \). To do this the expression \( \left[ I - AA^T W \right] TW \) in Equation 4.14 will be considered. Applying Equations 4.10 and 4.11 gives:

\[
\left[ I - AA^T W \right] TW = \left[ I - AA^T W \right] AA = AA - AA = 0
\]

(4.15)

This factor \( \left[ I - AA^T W \right] TW \) of the expression on the right hand side of Equation 4.14 is a matrix of zeroes which implies that \( \frac{ds}{dW_{k,k}} \) is zero for all values of \( k \). To show that this is a minimum and not a saddle point, it is necessary to show that the corresponding Hessian matrix, \( H \), is positive semi-definite.
The elements of the Hessian matrix, $H_{i,j}$, are given by:

$$H_{i,j} = u^T A A^T \frac{dW}{dW_{i,i}} [I - A A^T W] T \frac{dW}{dW_{j,j}} A A^T u \quad \text{(for } i, j = 1 \ldots q)$$

(4.16)

Using Equation 4.11 the matrix $[I - A A^T W] T$ can be expressed as:

$$[I - A A^T W] T = T - A A A^T$$

(4.17)

The $q \times q$ matrix $T - A A A^T$ is symmetric and it has $n$ zero eigenvalues where $n$ is the number of columns of the matrix $A$. To show that the matrix $T - A A A^T$ is positive semi-definite it is sufficient to show that its smallest nonzero eigenvalue, $\lambda_{\text{min}}(q, n)$, is positive for all values of $q$ and $n$. For the case where $n = 1$ the smallest nonzero eigenvalue is given by:

$$\lambda_{\text{min}}(q, 1) = 2 \left[ 1 - \cos \left( \frac{2\pi}{q+1} \right) \right] \quad \text{(for } n = 1, \ q = 2, 3, \ldots)$$

(4.18)

$\lambda_{\text{min}}(q, 1)$ is positive for all $q > 1$. If $q$ is fixed then the smallest nonzero eigenvalue increases monotonically as $n$ increases from 1 to $q - 1$. The value of $\lambda_{\text{min}}$ for $n = q - 1$ is given by:

$$\lambda_{\text{min}}(q, q - 1) = 4 - \frac{2}{q+1} - \frac{2}{\binom{q}{2}} \quad \text{(for } n = q - 1, \ q = 2, 3, \ldots)$$

(4.19)

where the parentheses on the right hand side denote a binomial coefficient. Therefore the smallest nonzero eigenvalue is in the range $0 < \lambda_{\text{min}}(q, n) < 4$ for all $q$ and $n < q$. This implies that the matrix $[I - A A^T W] T$ is positive semi-definite and can be factored as:

$$[I - A A^T W] T = R^T R$$

(4.20)

The matrix $S$ is defined as:

$$S = R \, \text{diag} \, (A A^T u)$$

(4.21)

where the diag operator transforms the elements of a vector into the elements of a diagonal matrix. With this the Hessian matrix, $H$, can be factored as:

$$H = S^T S$$

(4.22)

Therefore $H$ is positive semi-definite and the weight vector $w$, given by Equation 4.2, minimizes the smoothing parameter $s$.

The matrix $T$ has the property that $-T$ is the operator that acts on a vector to give the second differences of the vector. It can be seen from Equation 4.2 that $-T$ acts on the vector $w$ to yield $-v$, a vector of minus ones. This implies that the elements of the vector $w$ can be generated by a quadratic polynomial in the index $i$ whose leading term is $-i^2/2$. In fact the values of $w$ defined by Equation 4.2 are given by:

$$w_i = -\frac{i}{2} (i - q - 1) \quad \text{(for } i = 1 \ldots q)$$

(4.23)

This optimal weight function is a quadratic polynomial that is zero at one sample interval beyond the $q$ sample intervals, i.e.:

$$w_0 = w_{q+1} = 0$$

(4.24)
5 The Simplest Case of the S-G Filter

To compare the relative performances of the standard S-G filter with a constant weight function and the optimally weighted S-G filter with a quadratic weight function the case of the simplest S-G filter will be considered. In this case the fitting polynomial is just a constant. The matrix $X$ of Equation 2.2 is a column vector of ones and Equation 2.8 gives the filter coefficients:

$$c_i = \frac{1}{q} \quad (\text{for } i = 1 \ldots q) \quad (5.1)$$

This is the definition of a moving average filter with $q$ samples. The error reduction ratio (Equation 3.4) of the moving average filter is given by:

$$r_0 = \frac{\sigma_e^2}{\sigma_c^2} = \frac{1}{q} \quad (5.2)$$

where the subscript $\theta$ denotes a constant weight function. The smoothing parameter (Equation 3.8) of a moving average filter is given by:

$$s_0 = \frac{\sigma_{e}^{2}}{\sigma_{c}^{2}} = \frac{1}{q^{2}} \quad (5.3)$$

If Equation 2.10 is applied to a constant polynomial with the optimal weight function given by Equation 4.23 then the filter coefficients are:

$$c_i = \frac{6i(q+1-i)}{q(q+1)(q+2)} \quad (\text{for } i = 1 \ldots q) \quad (5.4)$$

These coefficients are simply a constant multiple of the optimal weights. The corresponding error reduction ratio is:

$$r_2 = \frac{6}{5} \frac{(q+1)^2 + 1}{q(q+1)(q+2)} \quad (5.5)$$

where the subscript $2$ denotes a quadratic weight function. The corresponding smoothing parameter is given by:

$$s_2 = \frac{6}{q(q+1)(q+2)} \quad (5.6)$$

The constant residual weight function of the standard S-G filter has the property of minimizing the error reduction ratio, $r$. Therefore it is not possible to select residual weights which will minimize both the error reduction ratio, $r$, and the smoothness parameter, $s$. The following two approximations illustrate the nature of the tradeoff for the case where the S-G fitting polynomial is a constant:

$$\frac{r_0}{r_2} \approx \frac{5}{6} \left(1 + \frac{1}{q}\right) \quad (\text{for } q > 5) \quad (5.7)$$

$$\frac{s_0}{s_2} \approx \frac{q}{6} \left(1 + \frac{3}{q}\right) \quad (\text{for } q > 3) \quad (5.8)$$

The error of these approximations approaches zero with increasing values of $q$. So as the sample size, $q$, increases the relative advantage of a constant weight function minimizing the error reduction ratio, $r$, approaches a constant whereas the relative advantage of a quadratic weight function minimizing the smoothness parameter, $s$, approaches proportionality to $q$. This asymmetry in the tradeoffs heavily favours optimizing the smoothing parameter, $s$, with a quadratic weight function rather than optimizing the error reduction ratio, $r$, with a constant weight function.
6 The General Case of the S-G Filter

For the general case of the S-G filter, fitting polynomials of degree higher than zero will be considered. However, the analysis here will be limited to the case where the middle element of the \( u \) vector of Equation 2.6 is chosen to be one, i.e., \( u_{(1+q)/2} = 1 \). It is this case for which the coefficient vector \( c \) is symmetric and the S-G filter is linear phase.

This case also has the counterintuitive property that only even polynomials need be considered in the derivation of the S-G filter coefficients. In this case the degree of the fitting polynomial is even. As before, \( n \) is the number of columns of the matrix \( X \) in Equation 2.2 where the \( j \)th column is \( x_{2j-2} \). It will also be convenient to denote the index of the middle element of the vector \( u \) by \( m \) so \( m = (1+q)/2 \) and \( u_m = 1 \).

Section 5 dealt with the simplest case of the S-G filter where the fitting polynomial is a constant. Even for this simplest case, Equations 5.5 and 5.6 for \( r_2 \) and \( s_2 \) are not simple. And these equations increase in complexity with increasing degree of the fitting polynomial. For the purpose of comparing the relative performance of the S-G filter with a constant and a quadratic weight function good approximations to the ratios \( r_0/r_2 \) and \( s_0/s_2 \) are adequate to illustrate how these ratios are influenced by the values of the filter parameters \( m \) and \( n \):

\[
\frac{r_0}{r_2} \approx 1 - \frac{(1 - \frac{n}{m})^2}{2(2n+1)} \quad (6.1)
\]

\[
\frac{s_0}{s_2} \approx 1 + \frac{3m(1 - \frac{n}{m})^2}{(2n+1)^2} \quad (6.2)
\]

For the case where \( m = n \) these approximations give the exact result that \( r_0/r_2 = s_0/s_2 = 1 \). In fact, in this case the S-G equations yield a degenerate solution where there is only one nonzero filter coefficient and the filter output is equal to the filter input. For a practical filter this imposes the constraint that \( m > n \). The conclusion drawn in Section 5 for the simplest case of the S-G filter where the fitting polynomial is a constant also holds for the general case of polynomials of any degree. The modest advantage of a constant weight function in the error reduction ratio, \( r \), is generally outweighed by a significant advantage of a quadratic weight function in the smoothness parameter, \( s \).

This result can also be interpreted in the frequency domain. The S-G filter cutoff frequency is very nearly proportional to the error reduction ratio, \( r \). Therefore the cutoff frequency is relatively insensitive to the choice of residual weight function while the frequency response in the stopband is much more sensitive to the choice of residual weight function [3].

For the sake of completeness, Turton’s use of a triangular residual weight function [3] will be considered. The triangular weight function, \( wt \), is given by:

\[
wt_i = 1 - \left| 1 - \frac{2i}{q+1} \right| \quad \text{(for } i = 1 \ldots q) \quad (6.3)
\]

If the smoothness parameter corresponding to this triangular weight function is denoted by \( s_1 \) then the filter smoothness parameter ratio, \( s_0/s_1 \), is approximated by:

\[
\frac{s_0}{s_1} \approx 1 + \frac{3m(1 - \frac{n}{m})^2}{(2n+3/2)^2} \quad (6.4)
\]

A comparison with Equation 6.2 giving the smoothness parameter ratio, \( s_0/s_2 \), for a quadratic weight function shows that the triangular weight function is very close to being optimal.
7 Conclusion

In his 1992 paper [3] Turton showed that applying a triangular residual weighting function in the derivation of the S-G filter significantly improves the frequency response of the S-G filter in the stopband. However Turton’s analysis has been largely overlooked in expository discussions of the S-G filter [2], [4], [5]. This paper has shown that a quadratic residual weight function optimizes a particular measure of filter output smoothness. While this may be an interesting theoretical result, it represents only a slight improvement over Turton’s choice of a triangular residual weight function.

The practical contribution of the present paper is in emphasizing the significance of Turton’s result with a time-domain analysis of the smoothing property of the S-G filter. Turton concluded his paper with this recommendation for the use of his variant of the S-G filter: “It should therefore be used in preference to the Savitzky-Golay filter in future spectroscopic applications.” The analysis presented here is offered in support of Turton’s recommendation.

References

[1] Savitzky, A. and Golay M.J.E. “Smoothing and differentiation of data by simplified least-squares procedures” Anal. Chem. 36 (1964) 1627-39
[2] Schafer, R.W. “What is a Savitzky-Golay filter?” IEEE Signal Process. Mag. July 2011, 111-117
[3] Turton, B.C.H. “A novel variant of the Savitzky-Golay filter for spectroscopic applications”.
       Meas. Sci. Technol. 3 (1992) 858-86
[4] Orfanidis, S.J. “Introduction to Signal Processing” Prentice Hall, 1995
[5] Press, W.H et. al. “Numerical Recipes, 3rd Ed.” Cambridge University Press, 2007