**Comparison and Optimization of Smoothing Procedures for Small-Angle X-ray Scattering Curves. Polynomial Fitting and Modified Frequency Filtering**

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**Abstract**

The filter theory allows one to compare the efficiencies of smoothing procedures widely used in the field of small-angle X-ray scattering. This method is demonstrated for polynomial fitting and modified frequency filtering. Optimized and objective smoothing parameters are determined for both procedures through the knowledge of variance reduction factors, transfer functions of the filters, the largest value of the spatial frequencies of the scattering curve and the distortions caused by the smoothing procedures. The comparison of the efficiency of polynomial fitting and frequency filtering clearly shows the superiority of the latter; therefore, this method has to be preferred.

**1. Introduction**

For reasons of intensity, small-angle X-ray scattering curves are mostly recorded by means of special scattering equipment with slit-like collimation of the X-ray primary beam (Kratky, Porod & Skala, 1960; Walter, Kranold & Becherer, 1974). In this way, the registered scattering curve $S(h)$ of a collimation distorted, a so-called smeared curve,

$$S(h) = G_1(h) \left\{ G_2(h) * \int_{-\infty}^{\infty} P(t) I[(t^2 + h^2)^{1/2}] dt + N(h) \right\}.$$  \hspace{1cm} (1)

$G_1(h)$ is a function equal to unity for all measured angular positions $h = 4\pi \sin \theta / \lambda$ ($2\theta =$ scattering angle, $\lambda =$ wavelength), and zero beyond the measured range. It describes the termination effects for very small and large scattering angles. $G_2(h)$ is the distribution of the intensity within the effective width profile of the primary beam. The folding procedure ($*$) describes the smearing caused by the beam width. The length smearing of the scattering curve $I(h)$ by the effective intensity distribution $P(t)$ in the length profile of the primary beam is calculated by the integral

$$J(h) = \int_{-\infty}^{\infty} P(t) I[(t^2 + h^2)^{1/2}] dt,$$  \hspace{1cm} (2)

t is a coordinate in the direction of the primary beam longitudinal profile and is measured in the same units as $h$. $N(h)$ is the random noise term. In general we have to calculate the scattering intensity with point collimation $I(h)$ from the smeared curve $S(h)$. Since this collimation correction procedure contains, explicitly or implicitly, a differentiation of experimental scattering curves, the various numerical procedures are extremely liable to statistical and nonstatistical errors. But as the small-angle scattering data are nearly always redundant (Damaschun, Müller & Pürschel, 1968; Oelschläger, 1969; Damaschun & Pürschel, 1969; Damaschun, Müller, Damaschun, Pürschel, Walter & Kranold, 1974), a numerical smoothing may precede the actual collimation correction procedure. There is a variety of numerical smoothing methods. Schmidt (1965) uses a curve-fitting procedure to fourth order polynomials, Dijkstra, Kortleve & Vonk (1966) introduced frequency filtering. Hossfeld (1968) fitted the curves by Hermite orthogonal polynomials. Damaschun, Müller & Pürschel (1971) developed frequency filtering to a practicable, physically based method and pointed out the adequacy of the method for the smoothing of curves with a range of the scattering intensity of more than three orders (Walter, Kranold, Müller & Damaschun, 1975). The fitting to $\sin ax / ax$ functions (Oelschläger, 1969), to spline functions (Schelten & Hossfeld, 1971), the matrix inversion method with reduction of the variables (Vonk, 1971), the recursive mean value calculation (Brämer & Wenig, 1972) and the implicit smoothing of difference curves (Glatter, 1974) are widely used methods to reduce the random noise. It is the purpose of this paper, based on the theory of digital filters (Wait, 1970; Kuo & Kaiser, 1966; Goldenberg, Lewtschuk & Poljak, 1974), to derive criteria allowing the various numerical methods to be compared and assessed by a uniform, theoretically based formalism. Furthermore, a modification of the frequency filtering (Wait, 1970; Wessel, 1978) of scattering curves is proposed which involves physically based smoothing parameters (Damaschun, Müller & Pürschel, 1971) and may serve as a suitable filter for smoothing slightly declining scattering curves (range of intensity $\sim 10^5$).

**2. Theory**

There are numerous and detailed reports on the theory of digital filters (Kuo & Kaiser, 1966; Wait, 1970; Goldenberg, Lewtschuk & Poljak, 1974). We now...
summarize the items essential for understanding the calculations.

2.1. Weighting function

An important role in the study of noise reduction and distortion of curves by a smoothing procedure (digital filter) is played by the so-called weighting function $b(j)$. For non-recursive digital filters, that is filters for which the smoothed values $\bar{y}_i$ are calculated only from unsmoothed values $y_i$, the smoothing instruction can be written according to Savitzky & Golay (1964) as

$$\bar{y}_i = \sum_{j=-M}^{M} b(j) y_{i+j}.$$  \hspace{1cm} (3)

In special cases $M_1 = M_2 = M$. The values $y_{i+j}$ are measured equidistantly, $2M + 1 = n$ is the number of curve points used for smoothing the $i$th value. The discrete values $b(j)$ satisfy the equation

$$\sum_{j=-M}^{M} b(j) = 1.$$  \hspace{1cm} (4)

For special functional systems such as polynomials (Savitzky & Golay, 1964), trigonometric functions (Damaschun, Müller & Pürschel, 1971), Hermite polynomials (Hossfeld, 1968), etc., $b(j)$ may be calculated by means of least-squares methods once for all. Smoothing then consists of a convolution of the scattering curve with the discrete function $b(j)$ according to equation (3). This avoids the necessity of performing least-squares procedures and provides accuracy and a saving of calculation time which is essential, especially when using computers with short word-length.

2.2. Variance reduction

The weighting function $b(j)$ is used to characterize the smoothing capabilities by a digital filter. A measure of the smoothing capabilities is the variance reduction factor $R$ (Monroe, 1962),

$$R = \frac{\sigma_3^2}{\sigma_2^2},$$  \hspace{1cm} (5)

if $\sigma_2$ is the variance in the experimental scattering curve

$$\sigma_2^2 = \sum_{i=1}^{K} \left[ S(h_i) - S_{\text{theor}}(h_i) \right]^2 / (K-1)$$  \hspace{1cm} (6)

and

$$\sigma_3^2 = \sum_{i=1}^{K} \left[ S_{\text{smoothed}}(h_i) - S_{\text{theor}}(h_i) \right]^2 / (K-1),$$  \hspace{1cm} (7)

the variance in the curve after smoothing. $K$ is the number of the experimental intensity values $S(h_i)$ with random noise, $S_{\text{theor}}(h_i)$ are the theoretical scattering intensities without any noise, and $S_{\text{smoothed}}(h_i)$ are the smoothed intensities. If the noise components at the sample points are completely unrelated, the factor $R$ can be calculated by equation (8),

$$R = \sum_{j=-M}^{M} b^2(j).$$  \hspace{1cm} (8)

2.3. Distortion by a filter

For qualitative appreciation of the systematic distortion caused by the digital filter, the transfer function $F(x)$ can be used. This function is calculated by a Fourier transformation according to equation (9) from the weighting function

$$F(x) = \sum_{j=-M}^{M} b(j) \cos (xj\Delta h),$$  \hspace{1cm} (9)

where $\Delta h$ is the angular increment.

To explain the meaning of transfer functions, the smoothing problem will be discussed in the so-called frequency domain of the scattering curve, that is in real space, denoted by the coordinate $x$. Smoothing of a curve in reciprocal space by equation (3) means a multiplication of the frequency function $C^*(x)$ of the scattering curve by the transfer function of the digital filter $F(x)$ in the real space. According to Damaschun et al. (1974), the frequency function of the scattering curve is calculated directly by Fourier-cosine-transformation of the experimental scattering curve. This frequency function is identical to the smeared auto-correlation function of the excess electron density $C(x)$,

$$\tilde{C}(x) = \int_{0}^{\infty} C[(x^2 + y^2)^{1/2}] dy,$$  \hspace{1cm} (10)

$$\hat{C}(x) = \frac{1}{\pi} \int_{0}^{\infty} J(h) \cos hx dh,$$  \hspace{1cm} (11)

for curves $J(h)$ measured by 'infinite slits' and is identical to the twofold smeared correlation function $\tilde{C}(x)$,

$$\tilde{C}_R(x) = \int_{0}^{\infty} C[(x^2 + y^2)^{1/2}] dy,$$  \hspace{1cm} (12)

$$\tilde{C}(x) = \frac{1}{\pi} \int_{0}^{\infty} I(h) \cos hx dh,$$  \hspace{1cm} (13)

for point collimation. $y$ is an integration variable with the same dimensions as $x$. The largest value $L$ of the spatial frequencies of the scattering system can be determined from the frequency function $C^*(x)$ (Damaschun et al., 1974). This value $L$ is equal to the largest diameter of the scattering inhomogeneities for samples with infinite dilution or to the range of order in the sample for finite dilution. In Fig. 1 the schematic frequency function $C^*(x)$ of a scattering curve is shown. For $x > L$ there exist only spatial frequencies caused by random noise. An ideal distortion-free transfer function of a digital filter would be a low pass

$$F(x) = \begin{cases} 1 & x \leq L \\ 0 & x > L. \end{cases}$$  \hspace{1cm} (14)

because the multiplication of the two functions $C^*(x)$ and $F(x)$ does not influence the spatial frequencies of the scattering system but removes all noise power within the spatial frequencies $x > L$. The greater the deviations of the transfer function from this ideal
rectangular function in the range \( x \leq L \), the more the frequency function \( C^*(x) \) is changed by the smoothing procedure, and consequently systematic distortions are produced in the scattering curve, as shown in § 3.2. In principle, the ideal low-pass cannot be used for experimental scattering curves with random errors (Bracewell, 1965), because \( C^*(x) \) will then not become identical with zero for \( x \geq L \) (Damaschun et al., 1974), and this discontinuity at \( x = L \) causes strong oscillations on the scattering curve. However, the ideal low pass must be changed only enough to avoid the discontinuities. Possibilities for this approximation will be discussed in §§ 3 and 4 in connection with polynomial fitting and modified Fourier series method.

2.4. The reduced sampling point distance

The increment \( \Delta h = (4\pi / 2) \Delta (\sin \theta) \) plays an important role in the choice of smoothing procedures, smoothing parameters and collimation correction procedures (\( 2\theta \) = scattering angle) (Walter, Kranold, Müller & Damaschun, 1975). To avoid scaling problems \( \Delta h \) is given below in multiples \( \beta \) of the sampling point distance \( 2\pi / 2L \). Thus we can write

\[
\Delta h = \beta 2\pi / 2L, \quad \beta \leq 1.
\]  

Then \( \beta \) is called the 'reduced sampling point distance'. When \( \beta = 1 \), each measuring point is a sampling point in the sense of the information theory, and smoothing without loss of information is impossible. If \( \beta < 1 \), the measurement is redundant and smoothing is possible without loss of information.

These theoretical considerations allow one to make an objective comparison of smoothing procedures with regard to their distortion of the scattering curve and noise reduction. In §§ 3 and 4 this will be done for polynomial fitting and modified frequency filtering. For polynomials, in § 3.3., we show that an objective choice of smoothing parameters by weighting and transfer functions and variance reduction factors is possible. Frequency filtering (Wait, 1970) is used in a modified form appropriate to smooth small-angle scattering curves whose intensity declines by less than three orders of magnitude.

3. Polynomial fitting

3.1. Weighting and transfer function for polynomials

Polynomial smoothing procedures were discussed by Savitzky & Golay (1964). From the variety of possible combinations of order \( p \) of the polynomial and the number \( n \) of the scattering points adapted to the polynomial we will deal here with polynomials of lower order, especially third order \( (p = 3) \),

\[
y = a_1 + a_2 h + a_3 h^2 + a_4 h^3,
\]  

where \( h \) is the equally spaced abscissa.

The smoothing for the \( i \)th curve point for a least-squares fit of a third order polynomial to \( n = 5 \) points is written as

\[
\tilde{y}_i = \frac{1}{3} \left[ -3y_{i-2} + 12y_{i-1} + 17y_i + 12y_{i+1} - 3y_{i+2} \right],
\]  

in agreement with equation (3). The weighting functions \( b(j) \) for fitting to 5, 7 and 9 equidistant curve points are drawn in Fig. 2. The transfer functions, calculated by equation (9), are shown in Fig. 3. The weighting functions agree for second and third order polynomials, as do the transfer functions. By an appropriate choice of the abscissa (Fig. 3) all the transfer functions are shifted into the same region irrespective of the number of sample points \( n \) and the reduced sampling point distance \( \beta \) used.

3.2. Distortions caused by a third-order polynomial

In order to reduce the amount of distortion of the scattering curve generated by the smoothing procedure

![Fig. 1. Schematic diagram of the frequency function \( C^*(x) \) of a scattering curve (---) and of the transfer function \( F(x) \) of an ideal low pass (--.--).](image)

![Fig. 2. Weighting function \( b(j) \) for both quadratic and cubic polynomials. \( j \) is the current number of the scattering points; the number \( n \) of scattering points being included in the smoothing procedure for one point: (●) 5; (x) 7; (O) 9.](image)
to a reasonable extent, \( n \) and \( \beta \) have to be selected such that the transfer function for \( x \leq L \) is not essentially different from unity. A general value of permissible deviation of the transfer function from unity is experimentally determined by test curves. We are dealing here with an extreme case; the noiseless, theoretical scattering curve \( I(h) \) of a sphere was submitted to the smoothing procedure. If \( n \) and \( \beta \) are chosen in such a way that for \( x = L \) the transfer function (Fig. 3) drops to 0.75 (\( n = 5, \beta = 0.45 \)), the relative distortion in the secondary maxima caused by the polynomial filter is about 10\%, and in the secondary minima varies from 100 to 1000\%. For a decrease of the transfer function to 0.95 (\( n = 5, \beta = 0.28 \)) the relative error in the secondary maxima is reduced to 2.5\% and in the minima to about 10 or 100\%. For \( n = 5, \beta = 0.1 \) and \( F(L) = 0.999 \), the relative errors caused by distortions are drawn in Fig. 4. The theoretical variance reduction factor calculated according to equation (8) is only 0.46 in the latter case (Fig. 5). The smaller the reduced sampling point distance, \( \beta \), is chosen for a given \( n \), the smaller are the deviations of the transfer function from unity \((x \leq L)\), and hence the distortion in the scattering curve. But the lower limit of \( \beta \) is set by the limited measuring time.

### 3.3. Variance reduction factor for low order polynomials

The variance reduction factor \( R \) for second to seventh-order polynomials as a function of \( \beta \) calculated according to equation (8) under the condition \( F(L) = 0.999 \) is shown in Fig. 5. The order \( p \) of the polynomial is the parameter. The variance reduction theoretically obtainable by an ideal low pass serves as a comparison curve. In Fig. 6 the variance reduction

![Fig. 3](image_url)

**Fig. 3.** Transfer function \( F(x) \) for both quadratic and cubic polynomials with the weighting functions \( h(n) \) shown in Fig. 2. The legend is the same as in Fig. 2.

![Fig. 4](image_url)

**Fig. 4.** Positive relative systematic deviation \((I - I_{\text{ideal}})100\%/I_{\text{ideal}}\) of a noiseless theoretical scattering curve of a sphere with radius \( R_k = 10 \) nm, \( \beta = 0.1 \) caused by digital filtering: (-----) caused by polynomial fitting, \( p = 3, F(L) = 0.999 \); (-----) caused by MFF, \( J\beta = 20 \); (----) scattering curve of the sphere.

![Fig. 5](image_url)

**Fig. 5.** Variance factor \( R \) for second factor \( R \) to seventh-order polynomials as a function of the reduced sampling point distance \( \beta \). The parameter is the order \( p \) of the polynomials: (O) \( p = 2,3 \); (x) \( p = 4,5 \); (Δ) \( p = 6,7 \); (----) ideal low pass. The arrows show the maximal \( \beta \) value for smoothing by the corresponding polynomial.
factor $R$ is plotted as a function of the number of points, $n$, to which the $p$th order polynomials are fitted. First we take from Fig. 5 the possible variance reduction $R$ for a $p$th order polynomial in accordance with the experimentally determined reduced sampling point distance $\beta$. We than use Fig. 6 to determine parameter $n$ which is optimal under these conditions.

This type of representation in Figs. 5 and 6 allows one to draw several conclusions:

(1) When using a $p$th order polynomial, $\beta$ must be less than the upper limit indicated by an arrow in Fig. 5, because otherwise the distortions in the smoothed scattering curves would exceed the amount determined for $F(L)=0.999$.

(2) For a given $\beta$ one can determine the factor $R$ for a $p$th order polynomial.

(3) If a certain smoothing capability $R$ is desired and there is in the computer software a special numerical filtering procedure of order $p$ it is possible to determine the necessary reduced sampling point distance $\beta$.

(4) The smaller the value of $\beta$ for given $p$ and $n$, the smaller are the distortions, or for a fixed distortion [e.g. by the condition $F(x)=0.999$], noise suppression is improved because the number of curve points $n$ that can be used for smoothing increases.

(5) The smoothing capabilities of polynomials of these orders (and low number of points $n$) for a given $\beta$ are much worse than those which could be obtained by means of an ideal low pass.

When the largest value $L$ of the spatial frequencies in the scattering curve and the reduced sampling point distance $\beta$ are known, after the choice of a reasonable distortion of the scattering curve, optimal and objective smoothing parameters $p$ and $n$ for polynomial curve fitting for a desired noise reduction can be obtained from Figs. 5 and 6. For larger values of $p$ and $n$ we have to make equivalent calculation. Application of polynomial smoothing to random noise will be made in § 5.

4. The modified frequency filtering procedure

4.1. Weighting and transfer function

While polynomial fitting is a least-squares convolution procedure in the scattering domain (reciprocal space), the smoothing in the frequency domain (real space) is based on the transfer function $F(x)$. The ideal low pass must be exchanged for a real one to avoid termination oscillations in the smoothed curve. Therefore an exponential tail for $x \geq L$ comes after the part $F(x)=1$ in the method of Damaschun et al. (1971, 1974). This tail influences only spatial frequencies in the frequency function $C^*(x)$ caused by random noise, but avoids the discontinuity and in general causes no distortions in the scattering curve. The smoothed curve is calculated by inverse transformation of the product of the transfer function $F(x)$ and $C^*(x)$, the Fourier transform of the scattering curve. Since this procedure works well only for scattering curves with an intensity decline of more than three orders, a modified frequency filter procedure (MFF) was adapted for our problems. The latter permits smoothing of curves with smaller variation in the intensity.

The smoothing procedure by means of the modified frequency filtering is performed in the scattering-curve domain, again according to equation (3) as in the least-squares methods. In the following section the weighting function $b(j)$ is calculated; the starting point is the transfer function $F(x)$ of the filter. To avoid the discontinuity in $F(x)$ which causes oscillations in the curve to be smoothed, the rectangular function of the ideal low pass is convoluted with a properly chosen function $W(x)$ with a small bandwidth. This convolution integral is the transfer function $F(x)$ of the filter. That means, in reciprocal space, the weighting function $b(j)$ obtained by Fourier transformation of $F(x)$ is the product of the Fourier transform $b_1(j)$ of the ideal low pass

$$b_1(j) = \sin (j\pi \beta)/(j\pi),$$

and the Fourier transform $H(j)$ of the function $W(x)$. An effective function $H(j)$ is the so-called Hamming's window function (Wait, 1970) in a modified form:

$$H(j) = \begin{cases} \cos^2 (j\pi/2J), & j \leq J \\ 0 & j > J. \end{cases}$$

(19)

For the weighting function we then have

$$b(j) = \begin{cases} \sin (j\pi \beta)/(j\pi)\cos^2 (j\pi/2J), & j \leq J \\ 0 & j > J. \end{cases}$$

(20)

$J$ is the window parameter; it indicates the number of scattering points included in the smoothing to the right and left of the point to be smoothed, $j$ is the current number of the data points measured at intervals $\pi\beta/L$. Fig. 7 shows the transfer functions $F(x)$ for this type of
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The parameter is the range Jβ. The larger Jβ, the broader the weighting function b(j) becomes, and more neighboring points are used for smoothing a single curve point and the function W(x), by which the low-pass transfer function is folded, becomes narrower.

4.2. Distortions by the modified frequency filtering procedure

The transfer functions approximate the ideal low pass very well for 10<Jβ<25 and the discontinuity at x/L = 1 is avoided. Only in a very narrow range in the neighborhood of the largest value L of the spatial frequencies is the frequency function C*(x) of the scattering curve changed when using this smoothing procedure; the systematic distortions remain low.

Substituting in equation (20) the experimental value β by the more convenient

\[ \beta' = \beta/[1 - 2/(\beta J)] \tag{21} \]

we have

\[ b(j) = \begin{cases} 
\sin\{j\pi[1 - 2/(\beta J)]\}/(j\pi\cos^2(j\pi/2J) \quad j \leq J \\
0 \quad j > J 
\end{cases} \tag{22} \]

and the transfer function F(x) is shifted in such a way as to drop to 0.999 (instead of 0.5) for an experimentally determined x = L. This reduces the distortions in the scattering curve further. The capability of noise reduction becomes somewhat worse of course, but these conditions are more convenient for practical use. For the theoretical scattering curve of a sphere with β = 0.1 (β' = 0.111) and βJ = 20, the relative deviations from the theoretical curve caused by the smoothing procedure amount to less than 0.1% (Fig. 4). This distortion is now small compared with the accuracy of experimental scattering curves.

4.3. Variance reduction by MFF

The variance reduction factor R for this smoothing procedure is depicted in Fig. 8. The parameter again is Jβ. For Jβ ≥ 10 the noise reduction becomes very close to the ideal case R = β. In practice the parameters are chosen for an optimized smoothing by means of the transfer function. The sole freely selectable smoothing parameter with an experimentally given scattering point distance Δh = β2π/(2L) is the window parameter J of Hamming's window. But this parameter is chosen to give a transfer function F(x) which does not produce systematic distortions and no significant oscillations greater than 0.1° in the curve to be smoothed. For noise amplitudes less than 10°, the parameter Jβ was found to be optimal within the interval 10 ≤ Jβ ≤ 25 by means of test calculations; the usual value of β is less than 0.25. A comparison of this method with polynomial fitting of scattering curves with random noise will show the superiority of the MFF procedure in many cases.

5. Smoothing of scattering curves with random noise

Let us now compare the MFF method with polynomial fitting for some test examples. Only calculations using third-order polynomials (n = 5) are made, higher orders guarantee better results but each set of p, n values needs a special computer program. As MFF is far better than polynomial fitting, and the coefficients b(j) in equation (3) are easy to calculate by means of equation (22) we will not discuss smoothing by higher polynomials. The test functions chosen are the same as selected by Walter, Kranold, Müller & Damaschun.
(1975) for discussion of desmearing problems. These examples are the scattering curves for coated spheres with the parameters: outer radius $R_o = 10 \text{ nm}$, inner radius $R_i = 6 \text{ nm}$, ratio of electron density within the core to that within the shell $Q_2/Q_1 = -4$, and secondly, $R_o = 2.6 \text{ nm}$, $R_i = 2.34 \text{ nm}$ and $Q_2/Q_1 = -0.9$ (Fig. 9).

The reduced sampling point distance was $\beta = 1/(2\pi)$, the superimposed random noise 3%. The relative noise amplitudes are shown in Fig. 10(a). The curves cannot be smoothed by polynomial fitting with the parameters $p = 3$, $n = 5$ and the secondary condition $F(L) = 0.999$. The scattering curve should therefore be measured with $\beta = 0.1$ and not with $\beta = 0.16$ as here for this amount of systematic distortion.

If polynomial fitting is formally applied, the theoretical noise reduction $R$ according to equation (8) is about 0.5. The value of $R$ calculated from equation (5) is of the same order but contains the systematic distortions. This smoothing for both scattering curves is insufficient [Figs. 10(b), (c)], the distortions cannot be detected because of the large amount of noise. The scattering curves, smoothed in this way and collimation corrected (desmeared) by Heine & Roppert's (1962) method, vary within an error band of 15% around the theoretical curves. MFF with the parameter $\beta J = 20$ gives a theoretical variance reduction of $R = 0.18$. The relative errors $[\hat{S}(h) - S(h)_{\text{theor}}]/S(h)_{\text{theor}}$ are also drawn in Figs. 10(b), (c); they are caused by noise frequencies $\chi < L$ and by distortions almost independently of the scattering curve. The slit-length collimation correction by Heine & Roppert (1962) produces desmeared curves within an error band of about 2% around the theoretical curves. Further test calculations with experimental scattering curves of biopolymers have shown that MFF is well suited for smoothing curves with a strong structure if the intensity falls by less than three orders. For example, the scattering curve of the enzyme yeast pyruvate decarboxylase (E.C.4.1.1.1.), is shown in Fig. 11. The reduced sampling point distance is $\beta = 0.11$, the smoothing parameter has been chosen to be $\beta J = 20$ and therefore the theoretically obtainable value for $R$ is 0.12.

6. Conclusions

While most of the smoothing procedures use empirical smoothing parameters, Damaschun, Müller & Pür-
ScheI (1968) have introduced the measurable largest value \( L \) of the spatial frequencies as an objective smoothing parameter. The theory of digital filters shows that the knowledge of \( L \) of a scattering curve to be smoothed is necessary, not only for frequency filtering methods but also for all other least-squares methods, if the smoothing procedure is to be optimized, that is if it gives the greatest possible noise reduction and the least distortion. The calculation of the variance reduction factor and the transfer function for smoothing procedures allow at once model-free comparisons for the capability to reduce noise and to smooth the scattering curve without large distortions. The MFF procedure proved to be the optimal method, rather than polynomial fitting. It is far better than low-order polynomial curve fitting with regard to the simplicity of handling, effectiveness in noise reduction and the insignificance of systematic distortions of the scattering curve. The use of the MFF procedure allows, with the same noise reduction, larger angular increments in comparison with a polynomial digital filter, or one can get a higher precision by means of MFF in the same measuring time. If a scattering curve was measured with \( \beta = 0.1 \), then a frequency filter \( (\beta J = 20, \beta^2 = 0.11) \) reaches a noise power reduction of \( R = 0.13 \) (Fig. 8).

For third-order polynomials, however, (Fig. 5) one obtains only \( R = 0.46 \) \((p = 3, n = 5)\). On the other hand, if a noise reduction of 0.46 is to be obtained, then the scattering curves with polynomial fitting \((p = 3, n = 5)\) have to be measured with a much smaller angular increment \((\beta = 0.1)\) than for frequency filtering \((\beta = 0.44)\). The distortion by the low-order polynomial filter is larger than for MFF as can be seen from the transfer functions in Figs. 3 and 7. The better smoothing quality of the MFF method in comparison with low-order polynomial fitting was shown by test examples. Since the sufficiency of MFF to smooth scattering curves with an intensity range less than \( 10^3 \) could be proved, and Walter, Kranold, Müller & Damaschun (1975) showed the fitness of the frequency filtering method of Damaschun, Müller & Pürschel (1971) for an intensity range larger than \( 10^3 \), optimized filtering procedures can be used with all kinds of scattering curves. In general, frequency filter methods require longer computation times than smoothing by low-order polynomials, because of the greater number of measuring points used to smooth a particular datum point. But since the smoothing algorithm for the MFF procedure according to equation (3) contains only additions and multiplications, the increase in computation time is insignificant. The frequency smoothing procedures in combination with the collimation correction method of Heine & Roppert (1962) provide desmeared scattering curves which oscillate in an error band around the theoretical curve as the experimental curve itself. Since the theoretically possible variance reduction \( R = \beta \) is almost reached with frequency filtering, noise reduction with model-free smoothing cannot be improved appreciably in comparison with the reduction achieved by these methods. However, it is possible to achieve a better smoothing by least-squares fits with a known structure of the scattering system. But this case will be the exception rather than the rule. An improvement in smoothing by further reduction of the systematic distortions may be possible by smoothing of difference curves (Glatter, 1972) if frequency-oriented smoothing methods with objective smoothing parameters are used.

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References


