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DECONVOLUTING SOURCE PULSE BROADENING IN PULSED SOURCE TIME-OF-FLIGHT MEASUREMENTS

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ABSTRACT

This paper describes the development of closed form expressions for deconvoluting several types of source pulse broadening, that due to double pulses, and those due to square-wave, triangular, and parabolic-shaped source pulses.

1. Introduction

An option exists within synchrotron design for first harmonic (h=1) or second harmonic (h=2) design. With h=1, single pulses will be delivered to the target at the system cycling frequency; with h=2, two pulses will be delivered per machine cycle, each of which would be narrower than the single h=1 pulse, but separated in time such that together the two pulses represent a broader pulse than that for h=1. The question is, which is more desirable from the standpoint of use by time-of-flight neutron scattering instruments. By way of background, operating pulsed spallation sources IPNS, KENS and LANSCE operate with single pulses, while ISIS operates in the double-pulse mode.

Narrow pulses are desirable from the point of view of instrument resolution; this makes a difference only in the range of higher neutron energies where the moderated pulse is intrinsically narrow. However, not to be ignored is that even for low neutron energies, the rising side of the pulse is quite sharp even though the falling side descends slowly from the peak. Therefore, judgments need to be made which respect the impact of proton pulse shape on the rise time of the moderated pulse, not simply on the basis of overall pulse width, since in this sense the shape of the proton pulse affects spectroscopy using even modestly low energy neutrons.

The general problem is one of deconvoluting broadening effects from measured data. Here, there are two effects to deal with, broadening due to the double pulse and broadening due to the time structure of individual pulses. The mathematical treatments of the two effects are similar, but the latter is substantially more complicated than the former. This paper draws no universal conclusions, however, the results can be used either to model specific cases or to perform model-independent deconvolutions of data. In this last sense, the results are complementary to maximum-entropy treatments.

Keywords: Deconvolution, Pulse broadening, Data treatment, Accelerator design

2. The General Problem

Say $C(t)$ is the observed counting rate at time t, $I(t)$ is the proton current at time t, $M(t)$ is the neutron current from the moderator at time t per unit of proton charge at time 0, and $R(t)$ is the counting rate in the detector of an instrument at time t after a neutron emerges from the moderator at time 0. Then, suppressing reference to certain details,

$$C(t) = I(t)*M(t)*R(t) \quad , \qquad (1)$$

where * represents convolution in time,

$$f(t) = g(t)*h(t) = \int_0^t g(\tau)h(t-\tau)d\tau \ . \qquad (2)$$

3. The Double Pulse Problem

Say protons appear as pairs of pulses of the same shape,

$$I(t) = i(t) + \alpha i(t-\delta) = H(\alpha,\delta;t)*i(t) \quad , \qquad (3)$$

where $i(t)$ describes the intensity distribution of one pulse, δ is the time delay between the first and the second pulses, and α is the ratio of the total charge in the second pulse to that in the first pulse. α and δ are known. $H(\alpha,\delta;t)$ is the double pulse function

$$H(\alpha,\delta;t) = \Delta(t) + \alpha\Delta(t-\delta) \qquad (4)$$

where $\Delta(x)$ is the Dirac delta function. (One expects $\alpha \approx 1$ but we carry $\alpha \neq 1$ for generality.) With appropriate definition of the time scale, causality arguments require $i(t) = I(t) = C(t) = M(t) = R(t) = 0$ for $t < 0$. All functions are well behaved for large t.

The response to a single pulse can be derived exactly from the response observed to the double pulse, for which we can write

$$C(t) = c(t) + \alpha c(t-\delta) = H(\alpha,\delta;t)*c(t) \quad , \qquad (5)$$

where $c(t)$ is the response to a single pulse

$$c(t) = i(t)*M(t)*R(t) \qquad (6)$$

and $c(t) = 0$ for $t < 0$. Equation (5) is a "difference equation"

$$c(t) = \begin{Bmatrix} C(t); & 0 < t \leq \delta \\ C(t) - \alpha c(t-\delta); & t > \delta \end{Bmatrix}. \qquad (7)$$

Thus $c(t)$ can be calculated sequentially starting from $t=0$, and could be computed and stored on the fly during measurement if desired. A closed form result for $c(t)$ in terms of

$C(t)$ can be derived trivially by induction from iterative use of (7) for sequential ranges of t, or elegantly by Laplace transform techniques[1]

$$c(t) = \sum_{n=0}^{[t/\delta]} (-\alpha)^n C(t-n\delta) \quad , \qquad (8)$$

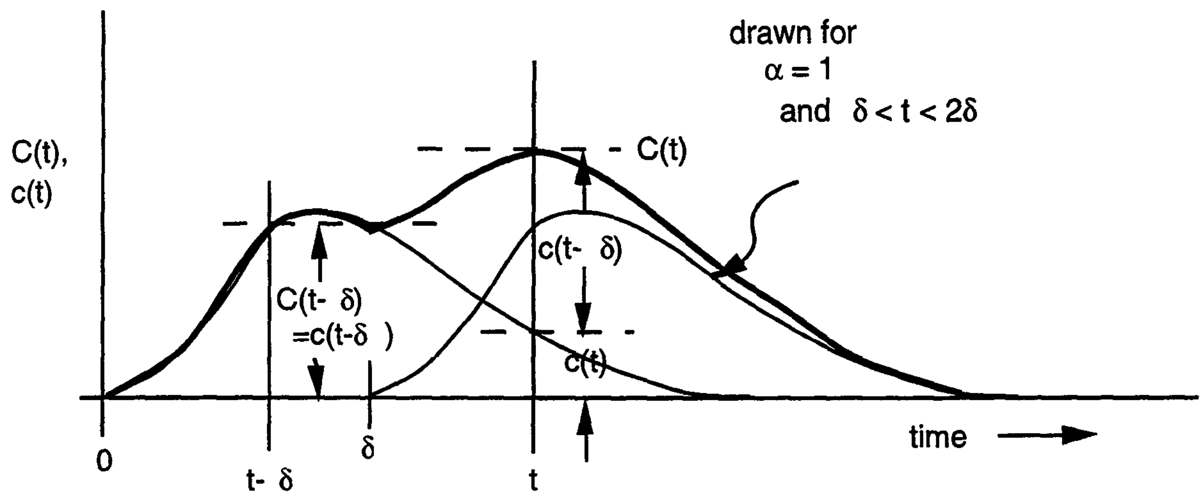
where $[t/\delta]$ is the greatest integer less than or equal to t/δ (e. g. $[1.9] = 1$). The result can also be expressed as a convolution in terms of a resolvent kernel

$$H^{-1}(\alpha,\delta;\tau) = \sum_{n=0}^{\infty} (-\alpha)^n \Delta(\tau-n\delta) \quad . \qquad (9)$$

Then

$$c(t) = \int_0^t H^{-1}(\alpha,\delta;\tau) C(t-\tau) d\tau \quad . \qquad (10)$$

The figure illustrates the situation for $\delta < t < 2\delta$.



The equations recorded so far are relationships among the expected values of measured functions. The measured values are subject to uncertainties, that is, they are statistically distributed quantities, but the expected-value relationships are always used to extract results from data. Assuming time binning on small time intervals so that t represents a discrete variable, then the statistical distribution of $C(t)$ for any time t is independent of the distribution of $C(t')$ for any other time $t' \neq t$. In particular, the distributions of the $C(t)$ are independent, Poisson-distributed counting errors. Extracted results $c(t)$ are also statistically distributed quantities but these typically have correlated errors. It will be necessary to deal with the results in these terms in order to come to conclusions concerning the effects of the double pulse and of the single pulse broadening of experimental results.

4. Pulse Shape Broadening

Now what can be said about the general problem of broadening due to the shape of the proton pulse $i(t)$? Recall

$$c(t) = i(t)*P(t) \quad , \qquad (6)$$

where we define

$$P(t) = M(t)*R(t) \quad . \qquad (11)$$

The object is to recover $P(t)$. Equation (6) is just an integral equation for $P(t)$, whose solution we seek. Such equations are Volterra integral equations of the first kind, with the special property that the kernel is a function of the difference between the inner and outer variables. Thus they are of the form of "faltung" (folding) integrals, formally amenable to solution by Laplace transform methods. The Laplace transform of (6) is

$$\tilde{c}(s) = \tilde{i}(s)\tilde{P}(s) \qquad (12)$$

where $\tilde{f}(s)$ is the Laplace transform of a function $f(t)$,

$$\tilde{f}(s) \equiv \int_0^{\infty} e^{-st} f(t)dt \quad . \qquad (13)$$

Then

$$\tilde{P}(s) = \frac{\tilde{c}(s)}{\tilde{i}(s)}, \qquad (14)$$

where ordinary division of functions is implied. Finally, formally, the result is the convolution, a faltung integral,

$$P(t) = i^{-1}(t)*c(t) \quad , \qquad (15)$$

where $i^{-1}(t)$ is the inverse Laplace transform of $\frac{1}{\tilde{i}(s)}$. $i^{-1}(t)$ may not be a well-behaved function but is expected to be an integrable density distribution. It turns out that this leads to problems in real cases such that it is not possible to express results in the form (15). In view of these complications of the Laplace inversion, we won't get much further without becoming specific about $i(t)$. Consider several cases, progressively more realistic.

4.1 Top Hat Distribution

$$i(t) = \frac{Q}{2b}\begin{cases} 1; & 0 \le t \le 2b, \\ 0; & t < 0, t > 2b \end{cases}, \qquad (16)$$

$$\tilde{i}(s) = Q\, e^{-sb} \left(\frac{\sinh(sb)}{sb}\right). \qquad (17)$$

4.2 Triangular Distribution

$$i(t) = \frac{Q}{2b}\left\{\begin{array}{ll} 1 - \left|\frac{t-2b}{2b}\right|; & 0 \le |t-2b| \le 2b \\ 0; & |t-2b| > 2b \end{array}\right\}, \qquad (18)$$

which is just (16) convoluted with itself. The transform

$$\tilde{i}(s) = Q\, e^{-2sb} \left(\frac{\sinh(sb)}{sb}\right)^2, \qquad (19)$$

is the square of (17). Having found the inversion function for the top hat distribution, the solution for the triangular distribution only involves convoluting the same function into itself, therefore we do not treat this case at any further length.

4.3 Parabolic Distribution

$$i(t) = \frac{3Q}{2b}\left\{\begin{array}{ll} 1 - \left(\frac{t-b/2}{b/2}\right)^2; & 0 \le t \le b \\ 0; & |t-b| > b \end{array}\right\} \qquad (20)$$

$$\tilde{i}(s) = 12Q\, e^{-sb/2} \left(\frac{(sb)\cosh(sb/2) - 2\sinh(sb/2)}{(sb)^3}\right). \qquad (21)$$

5. Worked Examples

5.1 The Top Hat Distribution

Taking the relatively simple top hat distribution as an example, the Laplace inversion of $\frac{1}{\tilde{i}(s)}$ gives

$$i^{-1}(t) = \frac{b}{Q}\int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} \frac{s e^{sb}}{\sinh sb}\, ds \qquad (22)$$

in which the integral is closed in the left half of the complex s-plane (standard Laplace transform theory.) A problem becomes clear, in that the integrand of (22) does not have the properties usually required of a Laplace transform; it is of order $|s|$ as $|s|$ becomes large, while, in order that it represent the transform of a well-behaved function, it must decrease more rapidly than $|s|^{-1}$ in that limit. Consequently any results gleaned from a formal pursuit of the inversion cannot be guaranteed.

We can obtain a result by differentiating the original equation, so that the top hat problem reduces to a particularly simple and familiar form; if $t > b$,

$$c(t) = \int_0^t i(\tau)P(t-\tau)\,d\tau = \frac{Q}{b}\int_0^b P(t-\tau)\,d\tau = \frac{Q}{b}\int_{t-b}^t P(u)\,du \qquad (23)$$

$$c'(t) \equiv \frac{dc(t)}{dt} = \frac{Q}{b}\left[P(t) - P(t-b)\right] \qquad (24)$$

and if $t < b$

$$c'(t) = \frac{Q}{b} P(t)\,. \qquad (25)$$

This is of the same form as the two pulse problem with $\alpha = -1$ and $\delta = b$ and the answer is of the same form,

$$P(t) = \frac{b}{Q}\sum_{n=0}^{[t/b]} c'(t - nb) \qquad (26)$$

although it involves the derivative $c'(t)$ rather than the function $c(t)$.

5.2 The Parabolic Distribution

The parabolic distribution (18) is a realistic description of the pulse broadening. Differentiation reduces the original problem to a simpler equation, but we are forced to more elegant methods than used above to obtain a result. We have

$$c'(t) = \int_0^t i'(t-\tau)P(\tau)d\tau \qquad (27)$$

where

$$i'(t) = 12\,\frac{Q}{b^3}\begin{Bmatrix} (b/2 - t);\ 0 \le t \le b \\ 0; \quad t > b \end{Bmatrix}. \qquad (28)$$

Twice more differentiating gives a difference-differential equation with constant coefficients that is tractable by Laplace transform methods

$$c'''(t) = 6\,\frac{Q}{b^2}\left[P'(t) + P'(t-b) - 2\,\frac{1}{b}\left(P(t) - P(t-b)\right)\right]. \qquad (29)$$

Since $P(-b) = P(0) = 0$, Laplace transformation gives

$$\widetilde{c'''}(s) = 12\,\frac{Q}{b^3}\left(\frac{sb}{2}(1 + e^{-sb}) - (1 - e^{-sb})\right)\tilde{P}(s)$$

$$\widetilde{c'''}(s) = 24\,\frac{Q}{b^3}\,e^{-sb/2}\left(\frac{sb}{2}\cosh sb/2 - \sinh sb/2\right)\tilde{P}(s)\,, \qquad (30)$$

familiar from (21). Thus

$$\tilde{P}(s) = \frac{b^3}{24Q} \frac{e^{sb/2}}{\left(\frac{sb}{2} \cosh sb/2 \; - \; \sinh sb/2 \right)} \widetilde{c'''}(s) \; . \qquad (31)$$

Inverting (32) as is leads to a slowly converging Fourier series which is difficult to recognize. However, the Laplace transform is similar to ones found in some problems of one dimensional heat flow[2] where a suggestive trick is used that produces a closed form result when we apply it here.

Write

$$\frac{e^z}{\left(z \cosh z \; - \; \sinh z \right)} = \frac{2e^z}{(z-1)(1 + \frac{z+1}{z-1} e^{-z})} \qquad (32)$$

which for large $Re\ z$, as required of the Laplace inversion, can be expanded

$$\frac{e^z}{\left(z \cosh z \; - \; \sinh z \right)} = \frac{2e^z}{z-1} \sum_{n=0}^{\infty} (-1)^n \left(\frac{z+1}{z-1} \right)^n e^{-nz} \; . \qquad (33)$$

Then the Laplace inversion becomes

$$f(b;t) = \frac{4}{b} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{\frac{2t}{b} z} \frac{e^z}{\left(z \cosh z \; - \; \sinh z \right)} dz =$$

$$= \frac{4}{b} \sum_{n=0}^{\infty} (-1)^n \int_{\gamma - i\infty}^{\gamma + i\infty} e^{\frac{2t}{b} z} \frac{(z+1)^n}{(z-1)^{n+1}} e^{-(n-1)z} dz \; . \qquad (34)$$

With the substitution $z \rightarrow z + 1$ this becomes

$$= \frac{4}{b} \sum_{n=0}^{\infty} (-1)^n e^{\frac{2t}{b} - (n-1)} \int_{\gamma' - i\infty}^{\gamma' + i\infty} e^{\left(\frac{2t}{b} - (n-1) \right) z} \left(\frac{(z+2)^n}{z^{n+1}} \right) dz \; .$$

(35)

Expanding the numerator

$$= \frac{4}{b}\sum_{n=0}^{\infty} (-1)^n e^{\frac{2t}{b} - (n-1)} \sum_{k=0}^{n} \binom{n}{k} 2^{n-k} \int_{\gamma' - i\infty}^{\gamma' + i\infty} e^{\left(\frac{2t}{b} - (n-1)\right)z} \left(\frac{1}{z^{k+1}}\right) dz ,$$

(36)

where $\binom{n}{k}$ is the binomial coefficient, leaves the simple inversion integral

$$\int_{\gamma' - i\infty}^{\gamma' + i\infty} e^{z\tau} \left(\frac{1}{z^{k+1}}\right) dz = \begin{cases} \tau^k/k! \,;\, \tau \geq 0 \\ 0 \,;\, \tau < 0 \end{cases} \equiv U(\tau)\tau^k/k! \tag{37}$$

so that

$$f(b;t) = \frac{4}{b}\sum_{n=0}^{\infty} (-1)^n e^{\frac{2t}{b} - (n-1)}\, U\!\left(\frac{2t}{b} - (n-1)\right) \sum_{k=0}^{n} \binom{n}{k} 2^{n-k} \left(\frac{2t}{b} - (n-1)\right)^k / k! \,. \tag{38}$$

The result is not as horrifying as it might at first seem, since the step function (37) limits the otherwise-infinite n-sum to a maximum $n \leq 2t/b + 1$, while the k-sum is only a finite series. Thus, finally,

$$f(b;t) = \frac{4}{b} \sum_{n=0}^{[2t/b + 1]} (-1)^n 2^n e^{2t/b - (n-1)} \sum_{k=0}^{n} \frac{1}{k!} \binom{n}{k} \left(\frac{2t/b - (n-1)}{2}\right)^k . \tag{39}$$

This result enables deconvolution of the parabolic pulse broadening from measured data,

$$P(t) = f(b;t)^{*}c'''(t) = \int_0^t f(b;\tau)c'''(t-\tau)d\tau \quad . \tag{40}$$

6. The Derivatives

The results above involve derivatives of observed data, $C'(t)$, $c'(t)$, and $c'''(t)$ which arise naturally when they refer to functions of the continuous variable. However, we refer to measured, binned data, that is, functions of a discrete variable so that, strictly, derivatives do not exist. However, finite differences of discrete data can represent derivatives as can derivatives of fitted functions. Say time binning is on equispaced intervals ε. Then, for example, the central finite difference representation of the derivative $c'(t)$ for interval t is

$$c'(t) = \frac{1}{2\varepsilon}\big(c(t+\varepsilon) - c(t-\varepsilon)\big) \tag{41}$$

and of the third derivative $c'''(t)$ is

$$c'''(t) = \frac{1}{(2\varepsilon)^3}\big(c(t+3\varepsilon) - 3c(t+\varepsilon) + 3c(t-\varepsilon) - c(t-3\varepsilon)\big), \tag{42}$$

which are linearly related to the $c(t)$. Similarly, the derivatives could be represented in terms of the coefficients of an unweighted sliding cubic polynomial fit to the nearby data,

$$c(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3 \quad , \tag{43}$$

$$c'(t) = a_1 \ , c'''(t) = 6a_3 \quad , \tag{44}$$

which lead to forms similar to (41) and (42), in general, for the n^{th} derivative,

$$c^{(n)}(t) = \sum_{t'} d^{(n)} c(t - t') \quad , \tag{45}$$

where the $d^{(n)}$s are constants which, with the range of summation depend on the specific choice of method of differentiation. Formally, at least, we can connect such methods of differentiation into the results above, in terms of differentiation operators

$$D^{(n)}(t) \equiv \sum_{t'} d^{(n)} \Delta(t - t') \tag{46}$$

so that

$$c^{(n)}(t) = \int_0^\infty D^{(n)}(t-\tau) c(\tau)\, d\tau \ . \tag{47}$$

7. Assembling the Results

From (40)

$$P(t) = \int_0^t f(b;\tau) c'''(t-\tau) d\tau \quad = \int_0^t f(b;\tau) \int_0^\infty D^{(3)}(t-\tau-\tau') c(\tau')\, d\tau d\tau'$$

$$= \int_0^\infty \left[\int_0^t f(b;\tau)\, D^{(3)}(t-\tau-\tau') d\tau \right] c(\tau')\, d\tau' \ . \tag{48}$$

Using this result, put in finite-interval form, it is possible to model the effects of recovering the desired function $P(t)$ from data $c(t)$ or similarly from $C(t)$ for different model functions representing different classes of measurements. That exercise remains to be done, but the results here provide the basis for that work.

8. References

[1] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, Tables of Integral Transforms, McGraw-Hill, New York, 1954. Volume 1, page 243, line 22.

[2] H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, Second Edition, Oxford University Press, 1986. See § 3.10, § 9.4, esp. §12.5 IV.