Folding a Gaussian into Theoretical Data

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Abstract

We construct an approximation to a δ-function using a Gaussian of full width at half-maximum \( w \). This approximate δ-function is used to model a measuring instrument. The Gaussian is folded into theoretical data and used to approximate the outcome expected when measuring the quantity described by the theory.

1 Method

Consider the function

\[
\delta(x, w) = A \exp(-x^2/\Delta^2)
\]

where

\[
A = \frac{1}{w} \sqrt{\frac{\log(16)}{\pi}} \quad \text{and} \quad \Delta = \frac{w}{\sqrt{\log(16)}}.
\]

Note that \( A\Delta = 1/\sqrt{\pi} \). The function \( \delta(x, w) \), which serves as a finite-width approximation to the δ-function, satisfies

\[
\int_{-\infty}^{\infty} \delta(x, w) \, dx = 1.
\]

Fig. 1 shows the approximation function.

Figure 1: Finite-width approximation \( \delta(x, w) \) to a δ-function. Case where \( w = 1 \).
Figure 2: A Gaussian of width $w = 2/3$ is folded into a wedge function, which is shown in black, to give the result shown in red.

If we let $\delta(x, w)$ describe the response of an instrument to a unit signal at value $x$, then the response $F(x, w)$ to a distributed signal with amplitude $f(x)$ will be

$$F(z, w) = \int_{-\infty}^{\infty} \delta(x, w) f(z - x) \, dx.$$  \hspace{1cm} (4)

We approximate the above integral using the trapezoidal rule. To make this rule tractable, we truncate the above integral at a point $x_m$ where

$$\int_{-x_m}^{x_m} \delta(x, w) \, dx = 0.9999$$  \hspace{1cm} (5)

This point is $x_m = 1.6521822525771246w$. Thus, we approximate

$$F(z, w) \approx \int_{-x_m}^{x_m} \delta(x, w) f(z - x) \, dx.$$  \hspace{1cm} (6)

We suppose that $f(x)$ is laid out on a grid $x_i = ih$, $i = 0 \cdots n$, and that $\delta(x, w)$ is laid out on a grid $x_i = ih$, $i = 0 \cdots m$. The trapezoidal rule gives

$$F[x, w] = h \left[ \frac{1}{2} (f[x_i - x_m] + f[x_i + x_m]) \delta[x_m, w] + f[x_i] \delta[0, w] \right.$$  
$$+ \sum_{j=1}^{m-1} (f[x_i - x_j] + f[x_i + x_j]) \delta[x_j, w] \right].$$  \hspace{1cm} (7)

We extend the array $f[x_i]$ from $i = 0 \cdots n$ to $i = -m \cdots n + m$ by adding subarrays of 0’s before and after the original array. In this way, the transformed array $F[x_i, w]$ will be defined everywhere on the original grid. As an example, we show the result of folding a Gaussian into a wedge function in Fig. 2.

In Fig. 3, we consider the bound-state contribution to the dynamic structure function for scattering at $\theta = 130^\circ$ of a 9000 eV photon from a Ti metal.
plasma at $T = 10$ eV. The black curve in the left panel shows the theoretical structure function and the red curve shows the theoretical prediction after a 10 eV instrumental width is folded in. The panel on the right shows the total structure function after folding in the Gaussian instrument function.