

ON FALTUNG AND CORRELATION OF FUNCTIONS AND THEIR APPLICATION IN PHYSICAL PROBLEMS

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ABSTRACT

This paper deals with a number of applications of the correlation and faltung functions, their Fourier transforms and their integrals. It is possible to show that various types of distortions produced by a recording instrument do not affect the value of the integral of the quantity recorded. This should be of great interest to designers of recording instruments. The advantage of using the F.T. in compounding probability distribution functions is pointed out with an illustration giving a short derivation of Kluyver's famous distribution for the problem of random walk in two dimensions by using this method. Finally, the relation of the correlation function to the Patterson function of a crystal structure is also pointed out.

1. INTRODUCTION

Two types of integrals occur in various problems in physics and probability theory, which may be represented in the following form:

$$\int_{-\infty}^{+\infty} g(x') h(x - x') dx' = f(x) = g \ast h(x) \text{ (say)}, \quad (1)$$

$$\int_{-\infty}^{+\infty} g(x') h(x + x') dx' = c(x) = g \ast h(x) \text{ (say)}. \quad (2)$$

The former is called the "Faltung" (folding) or "convolution" of the functions $g(x)$ and $h(x)$. The latter does not seem to have been recognised as a typical form. However, the term "correlation function" of $g(x)$ and $h(x)$ seems to be appropriate for it, as it is the integral of the product of the value of $g(x)$ at x' and of $h(x)$ with its origin shifted by $-x$ at x' .

Equations (1) and (2) can also be written in another equivalent form, namely

$$gFh(x) = \int_{-\infty}^{+\infty} g(x-x') h(x') dx' = hFg(x) \quad (3)$$

$$gCh(x) = \int_{-\infty}^{+\infty} g(x'-x) h(x') dx' \neq hCg(x) \quad (4)$$

It is the purpose of this paper to point out some of the properties of these functions and a few types of problems in which they find application.

Analogous to the notation of matrix theory, we may define the following functions related to a given (complex) function $f(x) = a(x) + ib(x)$:

$$\tilde{f}(x) ['f\text{-transpose-}x'] = f(-x) = a(-x) + ib(-x) \quad (5a)$$

$$f^*(x) ['f\text{-conjugate-}x'] = [f(x)]^* = a(x) - ib(x) \quad (5b)$$

$$f^\dagger(x) ['f\text{-dagger-}x'] = \tilde{f}^*(x) = a(-x) - ib(-x) \quad (5c)$$

It is clear that

$$\tilde{\tilde{f}}(x) = f^{**}(x) = f^{\dagger\dagger}(x) = f(x) \quad (6)$$

and that the four operations identity, transpose, star and dagger form a group of order four, isomorphous with the group $D_2 (\equiv C_2 \times C_2)$.

By far the most interesting properties of the faltung and correlation functions are concerned with their integral and Fourier transform (F.T.). We define the F.T. of the function $f(x)$ as

$$F(X) = \int_{-\infty}^{+\infty} f(x) e^{i2\pi X x} dx, \quad (7a)$$

with the inverse relation

$$f(x) = \int_{-\infty}^{+\infty} F(X) e^{-i2\pi X x} dX. \quad (7b)$$

Then, it follows that the F.T. of $\tilde{f}(x)$, $f^*(x)$ and $f^\dagger(x)$ are $\tilde{F}(X)$, $F^\dagger(X)$ and $F^*(X)$ respectively and their integrals are F , F^* and F^* respectively, where

$$F = F(0) = \int_{-\infty}^{+\infty} f(x) dx. \quad (8)$$

Using the above results, the following are readily proved:

$$gch = \tilde{g}h \quad (9)$$

$$hcg = \tilde{h}g = g\tilde{h} = \tilde{gch} \quad (10)$$

$$gch^* = (g^*ch)^* \quad (11)$$

$$g\tilde{f}h = g^*ch = hcg^* \quad (12)$$

In particular, the results shown in Table I are noteworthy. Here, $G(X)$, $H(X)$ are the Fourier transforms of $g(x)$ and $h(x)$ and G and H are their integrals. The results that $\int_{-\infty}^{+\infty} gth(x) dx = GH$ and $\int_{-\infty}^{+\infty} gch(x) dx = G^*H$ may be called the "Faltung integral theorem" and the "correlation integral theorem" respectively.

TABLE I

Fourier transforms and integrals of faltung and correlation functions

Correlation function	Equivalent expression as a faltung	Fourier transform	Integral
$\tilde{g}h$	$g\tilde{h}$	$G(X)H(X)$	GH
gch	$\tilde{g}h$	$\tilde{G}(X)H(X)$	GH
g^*ch	$g\tilde{f}h$	$G^*(X)H(X)$	G^*H
$g\tilde{f}h$	g^*ch	$G\tilde{f}(X)H(X)$	G^*H

The extension of these equations to higher dimensions can readily be made with the following definitions:

$$gfh(r) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} g(r') h(r - r') dr' \quad (13)$$

$$gch(r) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} g(r') h(r + r') dr'. \quad (14)$$

The Fourier transform is

$$F(R) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} f(r) e^{i2\pi R \cdot r} dr$$

with the inverse

$$f(\mathbf{r}) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} F(\mathbf{R}) e^{-2\pi i \mathbf{R} \cdot \mathbf{r}} d\mathbf{R} \quad (16)$$

All the results mentioned above are then valid if \mathbf{r} is replaced by \mathbf{r} and \mathbf{X} by \mathbf{R} .

So also, the concept of the faltung function can be extended to the faltung or convolution of any number of functions g_1, g_2, \dots, g_k . Writing the integral defining the faltung of $g_1(\mathbf{r})$ and $g_2(\mathbf{r})$ in the symmetrical form

$$g_1 \text{f} g_2(\mathbf{r}) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} g_1(\mathbf{r}_1) g_2(\mathbf{r}_2) d\mathbf{r}_1, \quad \mathbf{r}_1 + \mathbf{r}_2 = \mathbf{r}, \quad (17)$$

we have more generally

$$\begin{aligned} f(\mathbf{r}) &= g_1 \text{f} g_2 \text{f} \dots \text{f} g_k(\mathbf{r}) \\ &= \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} g_1(\mathbf{r}_1) g_2(\mathbf{r}_2) \dots g_k(\mathbf{r}_k) d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_k, \end{aligned}$$

with

$$\mathbf{r}_1 + \mathbf{r}_2 + \dots + \mathbf{r}_k = \mathbf{r} \quad (18)$$

It is then readily shown that

$$F(\mathbf{R}) = G_1(\mathbf{R}) G_2(\mathbf{R}) \dots G_k(\mathbf{R}), \quad (19)$$

or the F.T. of the faltung function is the product of the F.T.'s of the k individual functions.

We shall now consider the application of these functions to a variety of problems which occur in physics. These have been chosen with the idea of illustrating the types of such problems and no attempt is made to make them exhaustive.

2. MICROPHOTOMETER RECORD

Suppose we are scanning a series of lines on a photographic plate by means of a microphotometer, whose exploring beam has a finite width w (say). For convenience, let the plate be a positive print of a spectrum, so that $h(x)$ [Fig. 1 (a)] represents the true variations in the transmission. However, because of the finite width of the microphotometer spot, the record $\phi(x)$ [Fig. 1 (b)] will not be equally sharp. It is readily seen that $\phi(x)$ is the correlation function of g with h , i.e.,

$$\phi(x) = \int_{-\infty}^{+\infty} g(x') h(x + x') dx = g \text{f} h(x) \quad (1)$$

The interesting point is that the application of the correlation integral theorem gives

$$\int_{-\infty}^{+\infty} \phi(x) dx = \int_{-\infty}^{+\infty} g(x) dx \cdot \int_{-\infty}^{+\infty} h(x) dx \quad (2)$$

or Area under the curve in the record = w (area under the true curve) (3)

where w = width of the microphotometer beam [the intensity being scaled such that $g(x) = 1$ within this width]. Thus, in spite of the distortion in the shape of the lines, the *integrated value* obtained from the record is proportional to the correct value. In fact, from the correlation integral theorem, this is true even if the intensity distribution in the microphotometer spot is not uniform. Extending this idea to the individual lines in the record [Fig. 1 (b)], the *areas* under the different peaks would be exactly proportional to the *areas* under the corresponding peaks in Fig. 1 (a), even for an arbitrary shape of the function $g(x)$. Of course, the peaks should be resolved, so that effectively the area is the integral from $-\infty$ to $+\infty$.

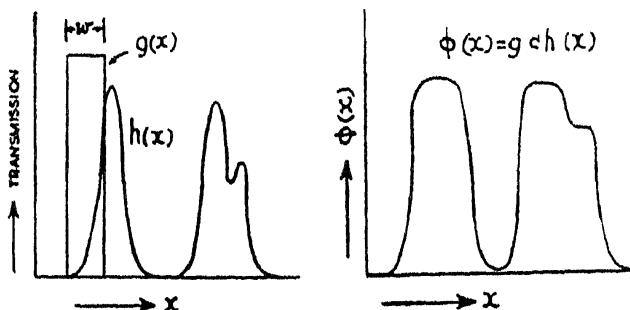


FIG. 1 (a)

FIG. 1 (b)

This result appears to the author to be important, for it is applicable to a variety of other cases, *e.g.*, in recording spectrophotometers and so on. It is obvious that if $h(x) = 1$ for all x , then $\phi(x) = \int g(x) dx =$ a constant K for all x . Then, Equation (2) becomes

$$\int_{-\infty}^{+\infty} \phi(x) dx = K \int_{-\infty}^{+\infty} h(x) dx. \quad (4)$$

Consequently, if the instrument is graduated to read unity for unit incident intensity when it is uniform, then the constant K becomes effectively unity, and thereafter all integrated values on the record will be correctly scaled automatically.

3. X-RAY REFLECTION WITH DIVERGENT BEAM

A problem which is mathematically very similar to the above is the shape (or angular distribution of intensity) of an X-ray reflection by a crystal, when the incident beam is not perfectly collimated.

Suppose $g(\theta)$ is the distribution of intensity about a mean position θ_0 when the incident beam has zero angular width [Fig. 2 (a)]. If $h(\theta'')$ is the angular distribution of intensity in the incident beam [Fig. 2 (b)], then it is obvious that the reflected intensity $R(\theta)$, when the crystal is set at $\theta_0 + \theta$, is

$$R(\theta) = \int_{-\infty}^{+\infty} g(\theta - \theta'') h(\theta'') d\theta'' = g \ast h(\theta). \quad (5)$$

A little reflection will show why the faltung integral occurs in this case, while the correlation integral occurs in the microphotometer problem. If the functions $f(x)$ and $g(x)$ are symmetrical, the two are one and the same, but they are not so in general.

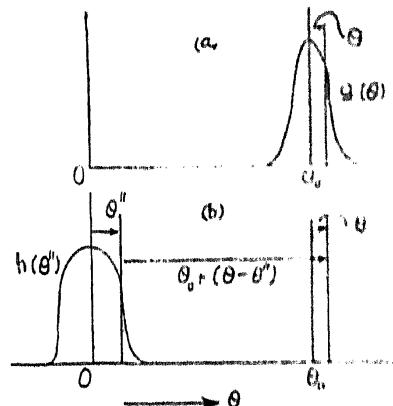


FIG. 2.

Just as in the previous case, an interesting result follows for the integral of $R(\theta)$. By the faltung integral theorem,

$$\int_{-\infty}^{+\infty} R(\theta) d\theta = \int_{-\infty}^{+\infty} g(\theta) d\theta \cdot \int_{-\infty}^{+\infty} h(\theta) d\theta = \rho E_0, \quad (6)$$

using a notation commonly used in crystallography.

i.e., $E_0 = \int h(\theta) d\theta$ is the total energy in the incident beam and $\rho = \int g(\theta) d\theta$ is the area under the curve $g(\theta)$ for perfect collimation, usually called the "integrated reflection". Thus,

$$\rho = \frac{\int R(\theta) d\theta}{E_0}, \quad (7)$$

and this is true, independent of the shapes of $h(\theta)$ and $g(\theta)$.

This Equation (7) is widely used by crystallographers and is usually derived for the case corresponding to Fig. 2 (a), i.e., for a perfectly collimated incident beam. However, in any experimental set-up, the incident beam has a finite angular width and the same formula is used for this case also. An intuitive justification of this may be given by supposing that the incident beam consists of a series of well-collimated components, for each of which the result (6) holds, so that it holds also for the sum. Going to the limit, Equation (7) follows. However, a rigorous justification for taking ρ to be equal to the ratio of the integrals of the observed reflection curve $[R(\theta)]$ to the total energy E_0 in the incident beam is only obtainable from the faltung integral theorem.

Incidentally, this shows that in any X-ray technique, irrespective of the shape of the line profile, the integrated intensity of the reflection is a true measure of the quantity ρ .

4. INTEGRATING METERS

(i) *Simple averaging.* Suppose $h(t)$ is the variation of some quantity say with time t , and suppose that a meter is able to register not this value, but only the mean value over the interval $t - \tau$ to $t + \tau$. This is the simplest type of integrating meter, for it gives a reading $\phi(t)$ proportional to the integral of $h(t)$ from $t - \tau$ to $t + \tau$. This can be written down immediately as a correlation function, by taking,

$$\begin{aligned} g(t) &= K \text{ for } -\tau \leq t \leq \tau \\ g(t) &= 0 \text{ outside this interval} \end{aligned} \quad (8)$$

and then

$$\phi(t) = K \int_{-\tau}^{\tau} h(t + t') g(t') dt. \quad (9)$$

As in the previous case, the meter can be made to give the correct value for a steady input by making $K = 1/2\tau$. In that case, it is seen that if a pulse is fed in, then the integrated value of the output is exactly equal to the integrated value of the input, although the shape of the output is distorted.

(ii) *Type of integration met with in counting rate meters.* Counting rate meters, used for instance with Geiger counters, contain a resistance-capacity tank circuit, to which charge is fed in at a rate proportional to the number of counts registered per second. Let $h(t)$ be this input current, so

that the amount of accumulated charge in time dt' at t is $h(t') dt'$. Since the tank circuit has a finite time constant $= CR$ (C = capacity, R = resistance), this charge will leak away exponentially as $e^{-\alpha(t-t')}$, where $\alpha = 1/CR$. Thus, the total charge at time t is

$$\int_{-\infty}^t h(t') e^{-\alpha(t-t')} dt' = f(t) \quad (\text{say}). \quad (10)$$

This can be put as a faltung function by defining

$$\begin{aligned} g(t) &= e^{-\alpha t} & \text{for } t \geq 0 \\ g(t) &= 0 & \text{for } t < 0 \end{aligned} \quad (11)$$

when

$$f(t) = gFh(t) = \int_{-\infty}^{+\infty} h(t') g(t-t') dt'. \quad (12)$$

The voltage across the condenser is obviously $V(t) = f(t)/C$ and so

$$V(t) = \frac{1}{C} gFh(t). \quad (13)$$

Consequently, if there is a sharp peak in the counting rate, and the true integrated value is $\int h(t) dt = H$, then the integral of the record, which is the voltage, is

$$\begin{aligned} \int V(t) dt &= \frac{1}{C} \int gFh(t) dt = \frac{1}{C} \int g(t) dt \cdot \int h(t) dt \\ &= \frac{H}{C} \int_0^{\infty} e^{-\alpha t} dt = \frac{H}{C\alpha} = HR. \end{aligned} \quad (14)$$

Thus, the integral of the recorded trace is exactly proportional to the integral of the input (H), the constant of proportionality being R . Once again, we find that the distortion of the shape of the peak does not matter and that the total area under the recorded curve is exactly proportional to the true value.

Incidentally, the absence of the capacity value (C) in HR of Eqn. (14) shows that, once the instrument is correctly calibrated, then the time constant can be altered by changing C , without affecting the calibration.

5. EFFECT OF DELAY WITH OR WITHOUT INTEGRATION

It is obvious that a simple delay cannot affect the integrated value of a quantity. Thus, if

$$f(x) = h(x - a).$$

then

$$\int_{-\infty}^{+\infty} f(x) dx = \int_{-\infty}^{+\infty} h(x - a) dx = H. \quad (15)$$

On the other hand, suppose there is a delay in recording in addition to integration in an integrating meter. Denoting the independent variable quite generally by x (this may be time or distance on a recording paper), the two effects together can be represented by the equation

$$f(x) = K \int_{-\infty}^{+\infty} h(x - x' + a) g(x') dx' = KgFh(x + a). \quad (16)$$

It is again clear that the integrated value of $f(x)$ will be proportional to the integrated value of $h(x)$.

These results can be generalised as follows: *Irrespective of any instrumental effects like integrating time, delay, etc., if a meter is calibrated to read correctly for constant input, the integral of the record will be correct even for varying input, i.e., there may be a large distortion in the record, but the integrated value will be correct.*

6. PROBABILITY DISTRIBUTION FUNCTIONS

The concept of the faltung of two or more functions occurs most frequently in the applications of probability theory. If $p_1(x_1)$, $p_2(x_2)$, ... $p_n(x_n)$ are the probability distribution functions* (p.d.f.) of a number of random variables x_i and if $x = \sum_1^n x_i$ and the variables are independent, then the p.d.f. of x is clearly

$$p(x) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} p_1(x_1) p_2(x_2) \dots p_n(x_n) dx_1 \dots dx_{n-1} \quad (17)$$

* The term distribution function is used here to denote the function $p(x)$, which gives the probability that the variable lies between x and $x + dx$ as $p(x) dx$. This agrees with the nomenclature in physics and applied mathematics (e.g., Maxwell distribution of velocities, Gaussian distribution of errors, etc.), besides being description of the actual function. It is a pity that in the more abstract studies on probability, the term "distribution" is used for the integral of this function, while the term "frequency function" is used for $p(x)$.

with

$$x = x_1 + x_2 + \dots + x_n. \quad (18)$$

Thus, $p(x)$ is the faltung of the n functions $p_i(x_i)$.

Proof that $p(x)$ is a p.d.f.—Mathematically, a p.d.f. $p_i(x_i)$ satisfies the following two conditions

$$\left. \begin{array}{l} (a) p_i(x_i) \text{ is positive for all } x_i \\ (b) \int_{-\infty}^{+\infty} p_i(x_i) dx_i = 1 \end{array} \right\}. \quad (19)$$

The range of integration may be finite in many cases, but it can always be made infinite by putting $p_i = 0$ outside this range.

Now Equation (17) may be derived by probability arguments and $p(x) dx$ then gives the probability that the compounded variable x lies between x and $x + dx$. However, the simplest proof that the function $p(x)$ defined by Equation (17) is in fact a p.d.f. and satisfies 19 (a) and (b) is obtained by an application of the faltung integral theorem. Then it follows that

$$\int_{-\infty}^{+\infty} p(x) dx = \prod_{i=1}^n \int_{-\infty}^{+\infty} p_i(x_i) dx_i = 1, \quad (20)$$

thus proving the condition 19 (a). The positivity condition (19 b) is obtained from the fact that all the terms occurring in Equation (17) are positive.

Now it immediately follows from Equations (17) and (18) that their F.T.'s are related by the equation

$$P(X) = P_1(X) \dots P_n(X) = \prod_{i=1}^n P_i(X). \quad (21)$$

In stochastic theory, $P(x)$ is called the characteristic function of $p(x)$ and Equation (19) may be then interpreted in the following form: "When a number of p.d.f.'s are compounded, the characteristic function of the compounded p.d.f. is the product of the characteristic functions of the individual ones."

The above results are readily extended to joint probability distributions in any number of variables.

Thus, if

$$r = r_1 + r_2 + \dots + r_n,$$

then

$$p(\mathbf{r}) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} p_1(\mathbf{r}_1) \dots p_n(\mathbf{r}_n) d\mathbf{r}_1 \dots d\mathbf{r}_{n-1} \quad (22)$$

and we have also

$$p(\mathbf{r}) = \int \prod_{i=1}^n P_i(\mathbf{R}) e^{i2\pi \mathbf{r}_i \cdot \mathbf{R}} d\mathbf{R} \quad (23)$$

where

$$P_i(\mathbf{R}) = \int p_i(\mathbf{r}_i) e^{i2\pi \mathbf{r}_i \cdot \mathbf{R}} d\mathbf{r}_i. \quad (24)$$

In fact, the F.T. is a convenient means of doing the compounding, either numerically or even theoretically. Thus, Equations (23) and (24) are directly applicable to the derivation of the distribution $\phi_n(\mathbf{r}) d\mathbf{r}$ for the position of a particle after it has suffered n random displacements, when the distribution function for each displacement is given (Theory of Random Flights, Chandrasekhar, 1943). Remembering that 2π is included in the exponent in our formulæ, the above equations give at once Equations (51) and (52) of Chandrasekhar's formulation. Chandrasekhar has in fact used the F.T. method to work out various results in the theory of random flights in three dimensions.

It can also be used to work out in a straight-forward manner the general formula for the problem of random walk in two dimensions. Suppose the i -th step is of length l_i . The problem is to find the probability $W_n(r) dr$ that one is at a distance between r and $r + dr$ from the origin after taking n steps in random directions. The function $p_i(\mathbf{r}_i)$ is then given by

$$p_i(\mathbf{r}_i) = \frac{1}{2\pi} \delta(|\mathbf{r}_i|^2 - l_i^2) \quad (25)$$

whose F.T. is just

$$P_i(\mathbf{R}) = J_0(2\pi R/l_i).$$

Hence, if $\phi_n(\mathbf{r}) d\mathbf{r}$ is the probability that the resultant displacement after n steps lies in an area $d\mathbf{r}$ at \mathbf{r} , then

$$\text{F.T. of } \phi_n(\mathbf{r}) = \prod_{i=1}^n P_i(\mathbf{R}) = \prod_{i=1}^n J_0(2\pi R/l_i), \quad (26)$$

so that

$$\begin{aligned}
 W_n(r) &= 2\pi r \phi_n(r) \\
 &= 2\pi r \int_0^\infty \int_0^{2\pi} e^{-i2\pi Rr \cos \phi} \prod_{i=1}^n J_0(2\pi R l_i) R dR d\phi \\
 &= 4\pi^2 r \int_0^\infty R J_0(2\pi Rr) \prod_{i=1}^n J_0(2\pi R l_i) dR. \tag{27}
 \end{aligned}$$

Putting $2\pi R = x$, this gives

$$W_n(r) = r \int_0^\infty x J_0(rx) \prod_{i=1}^n J_0(l_i x) dx, \tag{28}$$

which is identical with the well-known formula of Kluyver (1906) in the form given by Rayleigh (1919), usually obtained by a long derivation.

Fourier transform methods seem to be ideally suited not only for compounding distribution functions, but also for deconvoluting functions,* e.g., to get $h(x)$ from $gfh(x)$ when $g(x)$ is known. The method can be employed for numerical calculations with ease, since routine methods of calculating Fourier transforms are available and the latter have only to be multiplied or divided thereafter.

7. CORRELATION FUNCTION OF REAL FUNCTIONS

For a real function $f(x)$, $\tilde{F}(X) = F^*(X)$ and it follows that if both $g(x)$ and $h(x)$ are real functions, then

$$\text{F.T. of } gch(x) = G^*(X) H(X).$$

In particular, if g and h are the same function, the function $gch(x)$ may be called the "autocorrelation function" of g . Its Fourier transform is then equal to $G^*(X) G(X) = |G(X)|^2$. This function is of very great importance in X-ray crystallography and is known as the Patterson function $[P(x)]$ in that field. In fact, the properties of $P(x)$, which is the inverse Fourier transform of $|G(X)|^2$ and of $f(x)$ the falting which is the inverse Fourier transform of $G(X) H(X)$ have been extensively studied in connection with a study of crystal structures by Ramachandran and Raman (1959) and Raman (1959).

* The use of the F.T. for deconvoluting a function has been pointed out by Stokes (1948, 1955) in connection with the study of X-ray line profiles.