Representation of Experimental Data by Fourier Functions for Differentiation

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Abstract

A LEAST-SQUARES approximation routine has been developed to fit Fourier functions to a given set of experimental data in order to obtain the first and second spatial derivatives. It has been observed that a continuous fit can be obtained provided that the input data are given in the form of a smoothly varying periodic function. Furthermore, the number of terms of the expansion must be chosen such that first the fit, and then the two subsequent derivatives are optimized. The derivatives are judged to be optimum when they are free from rapid oscillations.

Contents

In physics and engineering, it is often required to differentiate the experimental data of one independent variable (spatial or time) once or twice. To this end, an empirical function – at least twice differentiable – must be fitted to the data.[1] Furthermore, the curve fit must perform filtering on the data.[2] In other words, it should discard the noise in terms of experimental scatter, while giving the best fit. It has been observed that these requirements can be met to a large extent with a least-squares (LS) fit approach using Fourier functions rather than polynomials, as it has been the common practice so far.[1] Here, by an application of the Fourier functions $\{1, \cos(jx), \sin(jx)\}, j = 1,2...,M$, in the LS sense, the Mth partial sum of the standard (infinite) series is meant. In addition, only the expansion for data of one independent variable (spatial or time) is considered.

Given a periodic function $f(y)$ at discrete points y_i such that $f_i = f(y_i)$, y being the independent variable, not necessarily spatial, it is possible to approximate $f(y)$ with the following Fourier expansion having a discrete number of terms, G_i:[3-5]

$$G_i = a_0/2 + \sum_{j=1}^{M} \{a_j \cos[2\pi(i-1)j/N] + b_j \sin[2\pi(i-1)j/N]\} \tag{1}$$

where $M \leq (N-1)/2$; N being the total number of equally spaced discrete points in one period of $f(y)$ over which the function is defined. N can be even or odd (an odd number of points is considered here), and $i = 1,2,...,N$. In this expression, the Fourier coefficients a_j and b_j are defined as follows:

$$a_j = (2.0/N) \sum_{i=1}^{N} f_i \cos[2\pi(i-1)j/N] \tag{2}$$

$$b_j = (2.0/N) \sum_{i=1}^{N} f_i \sin[2\pi(i-1)j/N] \tag{3}$$

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due to orthogonality of the Fourier functions. For $M \to \infty$, if the summations in Eqs. (2) and (3) are replaced with integrals, then the standard Fourier series representation of the continuously defined fuction $f(y)$ is obtained. In that case, $G(y)$ will uniformly and absolutely converge to $f(y)$ provided that $f(y)$ is continuous and $f'(y)$ is piecewise continuous in $[0,2\pi]$; $f(y)$ is periodic with period 2π, and $f(0) = f(2\pi)$ (Ref. 6, p. 112). If Eq. (1) is used with $M < (N-1)/2$, then an LS approximation to $f(y)$ can be obtained. In this case, the sum of the squared error is expressed as follows:

$$\delta_M^2 = \sum_{i=1}^{N} \left\{ f_i^2 - (N/2.0) \left[a_0^2/2 + \sum_{j=1}^{M} (a_j^2 + b_j^2) \right] \right\} \tag{4}$$

If all of the previously stated conditions on $f(y)$ and $f'(y)$ are satisfied, then $\lim_{M\to\infty} \delta_M^2 = 0$. Furthermore, it can then be shown that $G(y)$, the infinite Fourier series representation of $f(y)$, can be differentiated term by term and that $G'(y)$ converges to $f'(y)$ (Ref. 6, p. 116).

In the present study, Eqs. (1-3) were used in developing a routine to find an LS fit to a given set of experimental data. The purpose was to obtain the first and second derivatives of the data with respect to the independent variable. To this end, the algorithm given by Goertzel[7] to calculate the coefficients a_j and b_j has been found to be the most efficient. The details and a flowchart of the present routine can be found in Ref. 1, along with a suggested modification of the conventional σ factors of Lanczos.[4,5]

In using the outlined routine, two points have been observed to be important. The first point is associated with the condition of having the input data periodic. Not every set of experimental data to be differentiated would be periodic with period 2π. Hence, it is required that the actual experimental data be extended as a periodic function. To this end, the data can be made to define an even function $[f(y) = f(-y)]$, or an odd one $[f(y) = -f(-y)]$. Therefore, either a cosine series or a sine series expansion, respectively, is sufficient instead of Eq. (1). However, it is convenient to use the general form as in Eq. (1), since this form reduces to the partial sum of either a cosine or a sine series, if the input data define an even or an odd function, respectively. Moreover, the actual interval over which $f(y)$ has been made periodic must be changed to represent 2π. This change of interval is implicit in Eq. (1).

As an example of how the data can be extended as a periodic function, the turbulence kinetic-energy $(\overline{q^2} = \overline{u^2} + \overline{v^2} + \overline{w^2})$ profile at 42 cm from the inlet of an 8-deg conical diffuser is given here, when the flow at the inlet was a fully developed turbulent pipe flow. This diffuser is 72 cm long, and the local radius at the station where these data had been collected is 80.0 mm. The details of the experimental facilities and the corrections done on the data are described in Ref. 1. In order to obtain the expected pattern of the first spatial derivative $\partial\overline{q^2}/\partial y$ (where y is the distance from the wall along the radius), the actual experimental data had to be extended over four radii, having been multiplied by -1.0 after the first two radii, in order to define a smoothly varying periodic function at the

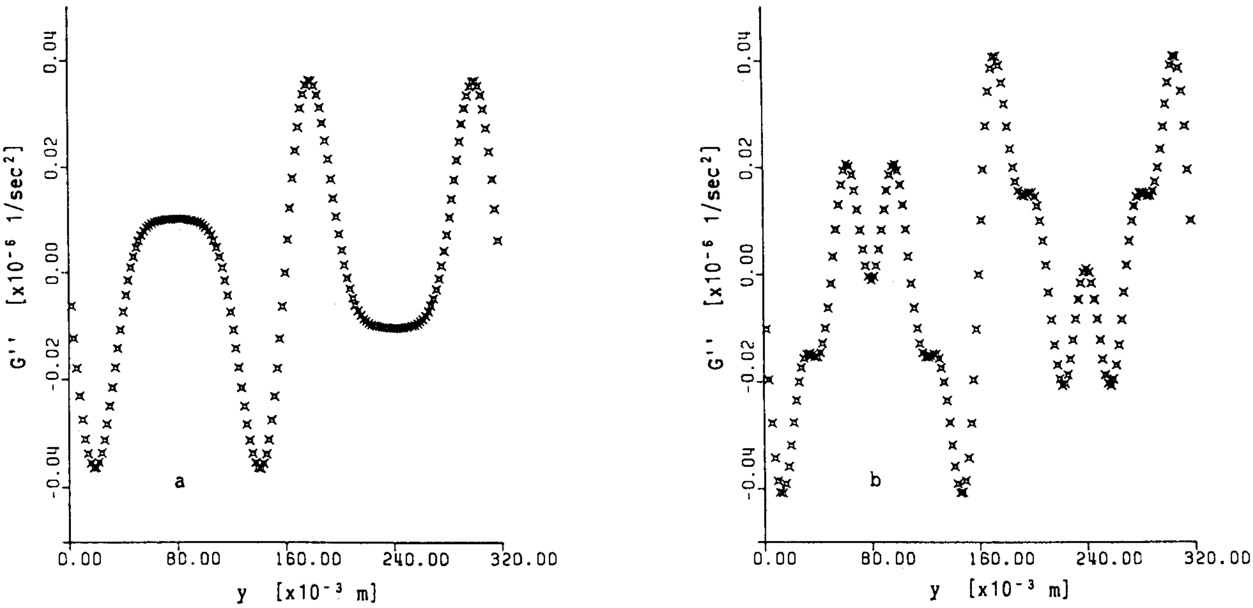

Fig. 1 Second derivative of the fitted function: a) $M=8$; b) $M=9$.

physical end points, $y = 0.0$ and $y = 160.0$ mm. It must be noted here that the actual experimental data can be extended as a periodic function using the boundary conditions at the end points, if there are any. The only boundary condition used here was that $\overline{q^2} = 0.0$ m²/s² at $y = 0.0$ mm. The other boundary conditions[8] governing the first and second spatial derivatives of $\overline{q^2}$ could not be used, because the experimental data were not available for $y < 2.0$ mm due to the size of the x-wire probes used.[1] As a result, the correct curvature of the experimental data was not known for $0.0 < y < 2.0$ mm, and hence, it was not possible to guess how the $\overline{q^2}$ profile tended to zero.

The second important point in using the present routine is the selection of the number of terms M to be used in the Fourier expansion to represent the input data. The decision on the magnitude of M can only be made by observing the plots of $G(y)$, $G'(y)$, and $G''(y)$ vs y. The fit to the function defines the lower limit of the number of coefficients to be used, i.e., the smallest value of M. As the value of M increases, the fit to the experimental data gets better, and hence, the value of δ_M^2 decreases, provided that the input data are extended to satisfy the previously stated conditions for uniform and absolute convergence. Therefore, the best fit to the given data is obtained for $\delta_M^2 = \delta_{M+1}^2 \sim 0$, excluding the cases for which this equality can be attained due to having either the even- or the odd-numbered coefficients of the expansion equal to zero. For such cases, $\delta_M^2 = \delta_{M+2}^2 \sim 0$ would be the criterion. However, even before either of these conditions can be satisfied, due to the contribution from high-frequency terms of the expansion, $G'(y)$ and $G''(y)$ become unacceptable. Therefore, the shape of the derivatives defines the upper limit of the value of M.

The procedure with which the value of M can be chosen is illustrated in Fig. 1. In this figure, the second derivative of the LS fit to the previously mentioned $\overline{q^2}$ data is given for $M = 8$ and $M = 9$. As seen in Fig. 1, unacceptable oscillations appear in the second derivative $\partial^2\overline{q^2}/\partial y^2$ for $M = 9$. Hence, $M = 8$ has been chosen as the acceptable number of coefficients to represent this set of data. The ratio δ_8^2/δ_9^2 is 1.18 for these two sets of coefficients.

In conclusion, if the input data can be defined as a continuous, smoothly varying periodic function even at the end points of the period, then a continuous LS fit – with continuous derivatives – to the given set of data can be obtained using Fourier functions. Although a priori knowledge of the order of the fit is not required, the number of terms of the expansion must be chosen by examining the plots of the fit to the data together with the plots of the corresponding first and second derivatives.

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