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# Exponential Approximations Using Fourier Series Partial Sums

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# EXPONENTIAL APPROXIMATIONS USING FOURIER SERIES PARTIAL SUMS

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**Abstract.** The problem of accurately reconstructing a piece-wise smooth, $2\pi$-periodic function $f$ and its first few derivatives, given only a truncated Fourier series representation of $f$, is studied and solved. The reconstruction process is divided into two steps. In the first step, the first $2N + 1$ Fourier coefficients of $f$ are used to approximate the locations and magnitudes of the discontinuities in $f$ and its first $M$ derivatives. This is accomplished by first finding initial estimates of these quantities based on certain properties of Gibbs phenomenon, and then refining these estimates by fitting the asymptotic form of the Fourier coefficients to the given coefficients using a least-squares approach. It is conjectured that the locations of the singularities are approximated to within $O\left(N^{-M-2}\right)$, and the associated jump of the $k^{th}$ derivative of $f$ is approximated to within $O\left(N^{-M-1+k}\right)$, as $N \to \infty$, and the method is robust. These estimates are then used with a class of singular basis functions, which have certain "built-in" singularities, to construct a new sequence of approximations to $f$. Each of these new approximations is the sum of a piecewise smooth function and a new Fourier series partial sum. When $N$ is proportional to $M$, it is shown that these new approximations, and their derivatives, converge exponentially in the maximum norm to $f$, and its corresponding derivatives, except in the union of a finite number of small open intervals containing the points of singularity of $f$. The total measure of these intervals decreases exponentially to zero as $M \to \infty$. The technique is illustrated with several examples.

**Key words.** Fourier series, exponentially accurate approximations, piecewise smooth functions, location of singularities

**Subject classification.** Applied and Numerical Mathematics

**1. Introduction.** Approximate solutions to problems in applied mathematics are often obtained using a finite number of terms in the Fourier series representation of the solution. In practice, this truncation procedure may lead to nonuniformly valid approximations. In particular, when the function being approximated has one or more points of discontinuity, Gibbs phenomena is present, resulting in an "overshoot" of the jump in the function at a point of discontinuity, as well as artificial oscillations near such a point. The magnitude of the overshoot is *not eliminated* by increasing the number of terms in the approximation. In addition, the oscillations caused by this phenomena typically propagate into regions away from the singularity, and, hence, degrade the quality of the partial sum approximation in these regions. It has been conjectured, however, that this oscillatory approximation, which may have been obtained by a high-order method, such as a spectral method, *should* contain enough information to enable the reconstruction of the proper, non-oscillatory, discontinuous function, by a post-processing filter (see, e.g., Lax [17]).

In a series of papers, Gottlieb, et. al. [7], [8], [9], [10], [11], have proposed and investigated a way of overcoming the Gibbs phenomena. Their technique involves the construction of a new series using the Gegenbauer polynomials. For a function $f$ that is analytic on the interval $[-1, 1]$, but is not periodic, they prove that their technique leads to a series which converges exponentially to $f$ in the maximum norm. Re-

cently, Geer [5] introduced and studied a class of approximations $\{F_{N,M}\}$ to a periodic function $f$ which uses the ideas of Padé approximations based on the Fourier series representation of $f$. Each approximation $F_{N,M}$ is the quotient of a trigonometric polynomial of degree $N$ and a trigonometric polynomial of degree $M$. It was proven that these "Fourier-Padé" approximations converge *point-wise* to $(f(x^+) + f(x^-))/2$ more rapidly (in some cases by a factor of $1/k^{2M}$) than the Fourier series partial sums on which they are based. Although these approximations do *not* "eliminate" Gibbs phenomena, they do mitigate its effect. In particular, the asymptotic value of the magnitude of the overshoot is reduced to about 6%, and, outside a "small" neighborhood of a point of discontinuity of $f$, the "unwanted" oscillations *can* (for practical purposes) be eliminated.

More recently, Geer and Banerjee [6] introduced a new, simple class of periodic "singular basis functions", which have special "built-in" singularities. They prove that these functions can be used to construct a sequence of approximations which *converges exponentially* to $f$ in the maximum norm. In particular, this implies that the Gibbs phenomena can be completely eliminated, even when $f$ has several points of discontinuity in the interval $[-\pi, \pi]$. In order to construct these approximations, the locations and magnitudes of the jumps in $f$ and its derivatives must be known a priori. For many applications, this may present a major limitation on the practical implementation of their method. However, an extension of their analysis shows that, *if sufficiently accurate approximations* to the locations and magnitudes of the discontinuities of $f$ can be obtained, then the singular basis functions can still be used to construct a sequence of approximations which *converges exponentially* to $f$ in the maximum norm, outside the union of a finite number of small, open sub-intervals containing the points of singularity.

The main purpose of this paper is to present and analyze a simple, accurate, and robust technique to estimate the points of singularity and the associated jumps in a Lipschitz function and its derivatives, given only a finite number of its Fourier coefficients. A number of other investigators, including Gottlieb, et. al. ([7], [8], [9]), Solomonoff [21], Eckhoff ([3], [4]) and Bauer [1], have investigated this problem, using a variety of approaches. In later sections, we shall compare our methods and results with theirs. After presenting our technique, we will illustrate how our estimates can be used with the singular basis functions method to accurately reconstruct the original (discontinuous) function, *as well as* its first few derivatives.

To fix notation, let $f$ be a $2\pi$-periodic Lipschitz function. Then $f$ has enough smoothness and regularity properties so that its Fourier series exists and converges to $(f(x^+) + f(x^-))/2$, for every $x \in [-\pi, \pi]$, i.e.,

$$\lim_{N \to \infty} F_N(x) = \frac{1}{2}\left(f(x^+) + f(x^-)\right), \quad F_N(x) \equiv \frac{a_0}{2} + \sum_{j=1}^{N} a_j \cos(jx) + b_j \sin(jx),$$

(1.1)
$$\begin{pmatrix} a_j \\ b_j \end{pmatrix} = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \begin{pmatrix} \cos(jx) \\ \sin(jx) \end{pmatrix} dx, \quad j = 0, 1, \dots .$$

Here $f(x^+)$ $(f(x^-))$ denotes the limit of $f$ from the right (left) at $x$, and $F_N$ denotes the $N^{th}$ Fourier series partial sum associated with $f(x)$.

We shall say that $x_0$ is a point of *simple discontinuity* of $f$ if

$$[f(x_0)] \equiv f(x_0^+) - f(x_0^-) \neq 0.$$

Also, we shall say that $x_0$ is a point of *contact discontinuity of order $q$* of $f$ if

$$\left[f^{(k)}(x_0)\right] = 0, \quad k = 0, 1, \dots, q-1, \quad \text{and} \quad \left[f^{(q)}(x_0)\right] \neq 0.$$

Here $f^{(k)}$ denotes the $k^{th}$ derivative of $f$, and, since we are assuming that $f$ is Lipschitz, both the left and right limits of each derivative of $f$ exist at every point in the interval $[-\pi, \pi]$. We call a point where $f$ has either a simple discontinuity or a contact discontinuity a point of *singularity* of the function.

We now assume that $f$ has a *finite* (unknown) number, $n$, of singularities which lie at the (unknown) locations $x_1$, $x_2$, ... , $x_n$ in the interval $(-\pi, \pi]$. The fundamental problem we shall address and solve in this paper is that of determining accurate and robust approximations of the singularity locations $\{x_s\}$ and the associated jumps $\left[f^{(k)}(x_s)\right]$, $k = 0, 1, ...$, *given only* the first $2N + 1$ Fourier coefficients $\{a_j, b_j\}$. In Section 2, we show how initial estimates of these quantities can be obtained for the simple discontinuities of $f$ (i.e., for $k = 0$), by capitalizing on certain properties of Gibbs phenomenon near these points. In Section 3, we formulate a least-squares optimization problem, which fits an asymptotic form of the Fourier coefficients, involving the points $\{x_s\}$ and $\{[f(x_s)]\}$, to some of the known coefficients. It is shown that this optimization problem can be solved efficiently, using the results of Section 2 as initial estimates. The result of this least-squares fit provides estimates of the singularity parameters of significantly higher quality than those obtained without the least-squares approach. In Sections 4 and 5, these results are extended to finding the jumps in $f'(x)$ at each point of simple discontinuity of $f$, as well as the locations and magnitudes of the first order contact discontinuities of $f$. In Section 6, these results are generalized to find discontinuities in the $M^{th}$ derivative of $f$, for $M \geq 2$. We shall refer to our method, including the determination of both initial and improved estimates of the singularity parameters, as the "least-squares parameter estimation" (LSPE) method. We compare our results with those of other investigators in Section 7. In Section 8, some aspects of the robustness of the LSPE method are discussed and illustrated with three examples. In Section 9, it is shown how the LSPE method can be used with the singular basis functions introduced in [6] to reconstruct the original (discontinuous) function, *as well as* its first few derivatives, with exponential accuracy. Some of the details of our analysis are included in two appendices.

**2. Points of simple discontinuity - initial estimates.** It is well known that, around a point, $x_s$, of simple discontinuity of $f$, the Fourier series partial sums $\{F_N\}$ exhibit Gibbs phenomenon. This phenomenon includes the oscillatory behavior of $F_N$ near $x_s$, as well as the tendency of $F_N$ to "overshoot" the magnitude of the jump in $f$ at $x_s$. The difference between the extrema of $F_N$ closest to $x_s$ asymptotically approaches about 118% of $[f(x_s)]$, as $N \to \infty$. Also, the locations of the extrema of $F_N(x)$, nearest to $x_s$, occur at $x = \eta_{s,\pm} = x_s \pm \pi/(N+1) + O(N^{-2})$, as $N \to \infty$. More precisely (see, e.g., Carslaw [2])

$$\lim_{N \to \infty} F_N\left(\eta_{s,\pm}\right) = \frac{f(x_s^+) + f(x_s^-)}{2} \pm \frac{1}{\pi} \operatorname{Si}(\pi)\left[f\left(x_s\right)\right],$$

and hence

$$(2.1) \qquad \lim_{N \to \infty} \left\{F_N\left(\eta_{s,+}\right) - F_N\left(\eta_{s,-}\right)\right\} = \frac{2}{\pi} \operatorname{Si}(\pi)\left[f\left(x_s\right)\right].$$

Here

$$\frac{2}{\pi} \operatorname{Si}(\pi) = \frac{2}{\pi} \int_0^\pi \frac{\sin(u)}{u} du \doteq 1.17898.$$

We now observe that, if we define a new sequence of partial sums

$$(2.2) \qquad D_N(x) = \frac{F_N\left(x + \pi/(N+1)\right) - F_N\left(x - \pi/(N+1)\right)}{(2/\pi)\operatorname{Si}(\pi)},$$

then, as $N \to \infty$, $D_N(x) \to 0$, if $f$ is continuous at $x$, but $D_N(x) \to [f(x_s)]$, if $x = x_s$ is a point of simple discontinuity of $f$. Thus, a simple method of identifying initial estimates of the points of simple discontinuity

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of $f$, as well as the corresponding jumps, is to find those points in the interval $(-\pi, \pi]$ for which the sequence $\{D_N(x)\}$ converges to a non-zero constant, as $N \to \infty$. At these points, $D_N$ exhibits peaks, which become narrower, with increasing $N$. More specifically, initial estimates of the points of simple discontinuity to $f$ can be obtained by locating the extrema, say $\tilde{x}_s$, of $D_N$, such that the corresponding values $D_N(\tilde{x}_s)$ do not tend to zero, as $N \to \infty$. For such a point, $D_N(\tilde{x}_s)$ provides an estimate of $[f(x_s)]$.

We now illustrate this idea with two examples.

**Example 1.** Let $f$ be defined by

(2.3)
$$f(x) = \begin{cases} 0, & 0 < x < 1, \\ 1 - x, & 1 < x < 3, \\ 5x^2 - 37x + 67, & 3 < x < 4, \quad , \quad f(x + 2\pi) = f(x). \\ x^3 - 15x^2 + 75x - 125, & 4 < x < 5, \\ 0, & 5 < x < 2\pi, \end{cases}$$

This function has only one point of simple discontinuity, namely, at $x_1 = 3$. However, it has multiple contact discontinuities; one of order 1 at $x_2 = 1$, one of order 2 at $x_3 = 4$, and one of order 3 at $x_4 = 5$. The jumps in $f$ and its derivatives at these points are summarized in Table 1.

| $\frac{Points \to}{Jumps \downarrow}$ | $x_2 = 1$ | $x_1 = 3$ | $x_3 = 4$ | $x_4 = 5$ |
|---|---|---|---|---|
| $[f(.)]$ | 0 | 3 | 0 | 0 |
| $[f'(.)]$ | $-1$ | $-6$ | 0 | 0 |
| $[f''(.)]$ | 0 | 10 | $-16$ | 0 |
| $[f'''(.)]$ | 0 | 0 | 6 | $-6$ |

Table 1: Exact locations and magnitudes of the discontinuities for Example 1.

A representative plot of $D_N(x)$ for this example is shown in Fig.1. By finding the extremum of $D_N$ closest to $x = 3$, we can estimate both the location and magnitude of the simple discontinuity of $f$ at this point. The absolute error in estimating the point of discontinuity, and the relative error in estimating the corresponding jump in $f$, using $D_N$, are summarized in Table 2 for several values of $N$. Also, in Figs. 2 and 3, we have plotted these errors (suitably normalized) as a function of $1/N$. These plots suggest that, using $D_N$, we can approximate the location of the simple discontinuity of $f$ with an error that is $O(N^{-2})$, and that we can approximate the associated jump with an error that is $O(N^{-1})$, as $N \to \infty$.

| $N$ | Absolute Error in $\tilde{x}_1$ | Relative Error in $D_N(\tilde{x}_1)$ |
|---|---|---|
| 16 | $3.2 \cdot 10^{-2}$ | $3.48 \cdot 10^{-1}$ |
| 32 | $9.4 \cdot 10^{-3}$ | $1.95 \cdot 10^{-1}$ |
| 64 | $2.6 \cdot 10^{-3}$ | $1.07 \cdot 10^{-1}$ |
| 128 | $6.8 \cdot 10^{-4}$ | $5.34 \cdot 10^{-2}$ |
| 256 | $1.7 \cdot 10^{-4}$ | $2.72 \cdot 10^{-2}$ |

Table 2: Errors in the initial approximations to the location and magnitude of the simple discontinuity in Example 1 using the partial sums $\{D_N(x)\}$.

**Example 2.** Let $f$ be defined by

$$(2.4) \qquad f(x) = \begin{cases} 0, & 0 < x < 1, \\ e^x, & 1 < x < 2, \\ \sin\left(\frac{x}{2}\right), & 2 < x < 5, \\ 0, & 5 < x < 2\pi, \end{cases} \qquad f(x + 2\pi) = f(x).$$

Here, $f$ has three points of singularity (with non-zero values of $\left[f^{(k)}(x)\right]$ at each of these points), and is analytic between these points. (This example has been used as a "benchmark" example by several other investigators. We will use it in later sections to compare our results with theirs.) The errors in locating the point of simple discontinuity at $x_1 = 1$, along with the errors in approximating the corresponding jump $[f(x_1)]$, are summarized in Table 3 for several values of $N$. The magnitude of the errors corresponding to the simple discontinuities at $x_2 = 2$ and $x_3 = 5$ are similar to those reported in Table 3. When these errors are plotted as functions of $1/N$, we obtain graphs that are qualitatively very similar to those shown in Figs. 2 and 3.

It can be shown that the rates of convergence of our approximations observed in these two examples hold in a more general setting. In Appendix A, we outline a proof of the following theorem, which establishes rigorously the rates of convergence of our approximations to $\{x_s\}$ and $\{[f(x_s)]\}$, as $N \to \infty$, using the partial sums $D_N(x)$.

| $N$ | Absolute Error in $\tilde{x}_1$ | Relative Error in $D_N(\tilde{x}_1)$ |
|-----|--------------------------------|--------------------------------------|
| 16  | $1.9 \cdot 10^{-2}$            | $1.8 \cdot 10^{-1}$                  |
| 32  | $6.6 \cdot 10^{-3}$            | $8.8 \cdot 10^{-2}$                  |
| 64  | $1.5 \cdot 10^{-3}$            | $4.2 \cdot 10^{-2}$                  |
| 128 | $3.6 \cdot 10^{-4}$            | $2.1 \cdot 10^{-2}$                  |
| 256 | $8.8 \cdot 10^{-5}$            | $1.0 \cdot 10^{-2}$                  |

**Table 3:** Errors in the initial approximations to the location and magnitude of the simple discontinuity at $x_1 = 1$ in Example 2 using the partial sums $\{D_N(x)\}$.

THEOREM 2.1. *Let $f(x)$ be a $2\pi$-periodic Lipschitz function with $n_0$ points $\{x_s\}$ of simple discontinuity in the interval $(-\pi, \pi]$. Then, as $N \to \infty$, the partial sums $D_N(x)$, defined in Eq.(2.2), converge to zero for all $x \neq x_s$, and converge to $[f(x_s)]$ at $x = x_s$. The point $\tilde{x}_s$, at which $D_N(x)$ attains its extremum in a neighborhood of $x_s$, approximates the point $x_s$ to within an error which is $O\left(N^{-2}\right)$, and the corresponding value $D_N(\tilde{x}_s)$ approximates $[f(x_s)]$ to within an error which is $O\left(N^{-1}\right)$, as $N \to \infty$.*

**3. Points of simple discontinuity - improved estimates.** We assume that the number $n_0$ of simple discontinuities of $f$, as well as initial estimates $\tilde{x}_s$ and $\tilde{J}_{0,s} = D_N(\tilde{x}_s)$ of $x_s$ and $[f(x_s)]$, respectively, for $s = 1, 2, ..., n_0$, have been obtained using the method of the previous section. We now show how to improve the quality of these estimates, by utilizing the asymptotic form of the coefficients $\{a_j, b_j\}$, expressed in terms of the parameters $\{x_s\}$ and $\{[f(x_s)]\}$, and a least-squares approximation technique.

The proof of the following lemma follows from the definitions (1.1) and by the repeated use of integration by parts (see, e.g., Kreyszig [14], pp. 489-493).

LEMMA 3.1. *Let $f$ be a $2\pi$-periodic Lipschitz function, with singularities at a finite number of points, say at $x = x_s$, $s = 1, ..., n$, in the interval $(-\pi, \pi]$. Then, for any non-negative integer $M$, the Fourier coefficients*

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*of f can be expressed as*

$$a_j = \frac{1}{\pi} \sum_{s=1}^{n} \left\{ \sin(jx_s) \left( \sum_{k=0}^{\lfloor M/2 \rfloor} \frac{(-1)^{k+1}}{j^{2k+1}} \left[ f^{(2k)}(x_s) \right] \right) \right.$$

$$\left. + \cos(jx_s) \left( \sum_{k=0}^{\lfloor (M-1)/2 \rfloor} \frac{(-1)^{k+1}}{j^{2k+2}} \left[ f^{(2k+1)}(x_s) \right] \right) \right\} + O\left(1/j^{M+2}\right),$$

$$b_j = \frac{1}{\pi} \sum_{s=1}^{n} \left\{ \cos(jx_s) \left( \sum_{k=0}^{\lfloor M/2 \rfloor} \frac{(-1)^{k}}{j^{2k+1}} \left[ f^{(2k)}(x_s) \right] \right) \right.$$

$$(3.1) \qquad \left. + \sin(jx_s) \left( \sum_{k=0}^{\lfloor (M-1)/2 \rfloor} \frac{(-1)^{k+1}}{j^{2k+2}} \left[ f^{(2k+1)}(x_s) \right] \right) \right\} + O\left(1/j^{M+2}\right),$$

*as $j \to \infty$. In the upper limits of the inner summations, $\lfloor q \rfloor$ denotes the greatest integer not exceeding $q$.*

We use Lemma 3.1 with $M = 0$ to write

$$j\pi a_j + \sum_{s=1}^{n_0} \sin(jx_s) \left[ f(x_s) \right] = O\left(j^{-1}\right),$$

$$(3.2) \qquad j\pi b_j - \sum_{s=1}^{n_0} \cos(jx_s) \left[ f(x_s) \right] = O\left(j^{-1}\right),$$

as $j \to \infty$, and then define a weighted least-squares error function

$$(3.3) \qquad E = E\left(\hat{x}_1, ..., \hat{x}_{n_0}, \hat{J}_{0,1}, ..., \hat{J}_{0,n_0}\right) \equiv \sum_{j=N+1-R}^{N} w_j \, E_j^{(0)},$$

$$(3.4) \qquad E_j^{(0)} \equiv \left( j\pi a_j + \sum_{s=1}^{n_0} \sin(j\hat{x}_s) \, \hat{J}_{0,s} \right)^2 + \left( j\pi b_j - \sum_{s=1}^{n_0} \cos(j\hat{x}_s) \hat{J}_{0,s} \right)^2.$$

Now, given the coefficients $\{a_j, b_j\}$, we seek to determine the values of $\hat{x}_1, \dots, \hat{x}_{n_0}, \hat{J}_{0,1}, \dots, \hat{J}_{0,n_0}$, say $x_1^*$, $\dots, x_{n_0}^*, J_{0,1}^*, \dots, J_{0,n_0}^*$, such that $E$ is a *minimum*, i.e.,

$$(3.5) \qquad \min_{\hat{x}_1, ..., \hat{J}_{0,n_0}} E\left(\hat{x}_1, ..., \hat{x}_{n_0}, \hat{J}_{0,1}, ..., \hat{J}_{0,n_0}\right) = E\left(x_1^*, ..., x_{n_0}^*, J_{0,1}^*, ..., J_{0,n_0}^*\right).$$

We note that, in order to have a true least-squares minimization problem, we must require that $R \geq n_0$, since there are $2n_0$ parameters to be estimated. However, we must also require that $N - R \gg 1$, in order for the asymptotic form of the Fourier coefficients to be valid. (We find the weighted least-squares strategy to be particularly useful when we assign larger weights to higher order terms defined in Eq.(3.3). This is due to the increasing accuracy of the asymptotic form (3.2) with the index $j$. )

From Eqs.(3.2)-(3.5), it follows that $x_s^* \to x_s$ and $J_{0,s}^* \to [f(x_s)]$, for $s = 1, ..., n_0$, as $N \to \infty$. More precisely, for the case $w_j = 1$, it follows from these equations that

$$x_s^* = x_s + \frac{[f'(x_s)]}{[f(x_s)]} \cdot \frac{1}{N^2} + O\left(1/N^4\right), \quad \text{and}$$

(3.6)
$$J_{0,s}^* = [f(x_s)] - \frac{[f''(x_s)]}{N^2} + O\left(1/N^3\right), \quad \text{as } N \to \infty.$$

Thus, the parameters we wish to estimate have now been characterized as the solution to a certain optimization problem. We shall demonstrate in later chapters that this formulation offers some nice advantages over the approaches used by several other investigators. In particular, we can see, at least intuitively, that the approximations determined by this approach should be less sensitive to "small errors" in the coefficients $\{a_j, b_j\}$, due both to the least-squares nature of the problem, and to the fact that the definition of $E$ "averages" over several (i.e., $2R$) coefficients.

To perform the minimization required by Eq.(3.5) in an efficient manner, we use the estimates obtained by the method of Section 2 as initial estimates for the nonlinear weighted least-squares method of Levenberg-Marquardt ([18], [19], [20]). Although the function in Eq.(3.5) can be minimized using a general unconstrained optimization technique, the special structure of the gradient, the Hessian matrix, and the general least-squares nature of $E$ is exploited by the Levenberg-Marquardt method. In choosing an optimization method, it is important to note that $E$ is a *badly scaled* objective function, which exhibits highly oscillatory behavior in some directions and very smooth, slowly changing behavior in other directions. In particular, a "flat" region of $E$ creates a problem for derivative based methods, because of the closeness of the derivatives to zero in that region. To illustrate this behavior, in Fig.4 we have plotted $E$ for Example 1 as a function of $\hat{x}_1$ and $\hat{J}_{0,1}$, near the minimum of $E$. In the figure we have set $N = 32$ and $R = 12$. For smaller values of $R$, the oscillations in the $\hat{x}_1$ direction are even more pronounced. The problem of the ill-conditioned associated Hessian matrix for $E$ can be partially mitigated by assigning larger values to the weights $w_j$, with increasing index $j$, in Eq.(3.3).

From these observations, it is important to note that we require *good* initial estimates of $\{x_s\}$ and $\{[f(x_s)]\}$ to initialize the search technique. Fortunately, the initial estimates obtained using the method based on the partial sums $D_N$, described in Section 2, are *good* and, in fact, are even better than we actually require. For example, from the definition of $E$ (see, also, Fig.4) we see that the width of each "valley" in the $\hat{x}_s$-direction is $O(1/N)$. Thus, to begin a search in the "proper valley", the initial estimate of each $\hat{x}_s$ should lie within a distance that is at least $O(1/N)$ of $x_s$. From Theorem 2.1, we see that our initial estimates lie within a distance which is $O(1/N^2)$ of $x_s$.

To illustrate this method, we again consider Examples 1 and 2. For Example 1, we use the initial estimates obtained in Section 2, whose errors are shown in Table 2, as starting values for the weighted least-squares method. The errors in the approximations to the discontinuity location $x_1 = 3$, and the corresponding jump in $f$, are summarized in Table 4 for several values of $N$, and are plotted (with suitable normalization) in Figs. 2 and 3. In Eq.(3.3), each $w_j = j$.

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| $N$ ($R$) | Absolute Error in $x_1^*$ | Relative Error in $J_{0,1}^*$ |
|---|---|---|
| 16 (8) | $1.14 \cdot 10^{-3}$ | $1.02 \cdot 10^{-2}$ |
| 32 (12) | $2.7 \cdot 10^{-3}$ | $2.45 \cdot 10^{-3}$ |
| 64 (15) | $6.05 \cdot 10^{-4}$ | $2.91 \cdot 10^{-4}$ |
| 128 (20) | $1.45 \cdot 10^{-4}$ | $4.86 \cdot 10^{-5}$ |
| 256 (28) | $3.38 \cdot 10^{-5}$ | $2.45 \cdot 10^{-5}$ |

**Table 4:** Errors in the estimates using the LSPE method of the location and magnitude of the simple discontinuity for Example 1.

Tables 4 and 2, as well as Figs. 2 and 3, illustrate that our approximations to both the location of the discontinuity and the associated jump have improved. In particular, they illustrate that, using the optimization idea, the order of the approximation to $x_1$ remains $O(N^{-2})$, but with a smaller proportionality constant. (Using Eqs.(11) and Eq.(A.9) of Appendix A, we see that this constant is smaller by a factor of $(\pi \, \mathrm{Si}(\pi))^{-1} \doteq 0.172$.) The order of the error in the associated jump in $f$ has improved from $O\left(N^{-1}\right)$ to $O\left(N^{-2}\right)$.

For Example 2, we again use the estimates from Section 2, whose errors are given in Table 3, to start the weighted least-squares method. The errors in the discontinuity location $x_1 = 1$, and the corresponding jump, for different fixed values of $N$, are summarized in Table 5. The order of the errors for the discontinuities at $x_2 = 2$ and $x_3 = 5$ are similar.

| $N$ ($R$) | Absolute Error in $x_1^*$ | Relative Error in $J_{0,1}^*$ |
|---|---|---|
| 32 (12) | $1.59 \cdot 10^{-3}$ | $2.93 \cdot 10^{-3}$ |
| 64 (15) | $3.1 \cdot 10^{-4}$ | $5.96 \cdot 10^{-4}$ |
| 128 (20) | $7.22 \cdot 10^{-5}$ | $9.52 \cdot 10^{-5}$ |
| 256 (28) | $1.63 \cdot 10^{-5}$ | $3.04 \cdot 10^{-5}$ |

**Table 5:** Errors in the estimates using the LSPE method of the location and magnitude of the simple discontinuity at $x_1 = 1$ for Example 2.

### 4. Discontinuities in $f'(x)$ - initial estimates.

To find initial estimates of the discontinuities in $f'$,

we are tempted to apply the method of Section 2 directly to the differentiated Fourier series partial sums. However, due to the presence of simple discontinuities in $f$, the differentiated Fourier series does not converge in a neighborhood of these points. Lanczos' ([16], pp. 61 - 74) "sigma factor smoothing" provides one way to mitigate this problem, but not to overcome it. The modification of the Fourier coefficients by the sigma factors causes the differentiated series to converge at all points where $f'(x)$ is finite. However, even after smoothing, the series diverges at all points where the derivative of the original function does not exist.

We now show that a slight modification and extension of the method based on the partial sums $\{D_N\}$, described in Section 2, can give us initial estimates of the discontinuities in $f'$ which are sufficiently accurate for our purposes. To see how this can be done, we use the (improved) estimates $\{x_s^*, J_{0,s}^*\}$ obtained in the previous section to define a new sequence of Fourier coefficients $\left\{a_j^{(0)}, b_j^{(0)}\right\}$ by

$$(4.1) \qquad a_j^{(0)} = a_j + \frac{1}{\pi j} \sum_{s=1}^{n_0} J_{0,s}^* \sin(j x_s^*), \quad b_j^{(0)} = b_j - \frac{1}{\pi j} \sum_{s=1}^{n_0} J_{0,s}^* \cos(j x_s^*),$$

for $j = 1, 2, ..., N$. (Intuitively, all we are doing here is "subtracting off" our best estimate of the parts of the

coefficients related to the simple discontinuities of $f$.) We then define a new sequence of partial sums

$$F_{1,N} = \frac{d}{dx} \sum_{j=1}^{N} \left\{ a_j^{(0)} \cos(jx) + b_j^{(0)} \sin(jx) \right\}$$

(4.2)
$$= \sum_{j=1}^{N} \left\{ a_j^{(1)} \cos(jx) + b_j^{(1)} \sin(jx) \right\},$$

$$a_j^{(1)} \equiv j b_j^{(0)}, \quad b_j^{(1)} \equiv -j a_j^{(0)},$$

which we can think of as the derivative of our original partial sum, but with the effect of the simple discontinuities "subtracted off". The coefficients in $F_{1,N}$ have the asymptotic form

$$a_j^{(1)} = \frac{1}{\pi} \left( \sum_{s=1}^{n_0} \cos(jx_s) \left[ f(x_s) \right] - \sum_{s=1}^{n_0} \cos(jx_s^*) J_{0,s}^* \right)$$

(4.3)
$$- \frac{1}{\pi j} \sum_{s=1}^{n_1} \sin(jx_s) \left[ f'(x_s) \right] + O\left( j^{-2} \right),$$

$$b_j^{(1)} = \frac{1}{\pi} \left( \sum_{s=1}^{n_0} \sin(jx_s) [f(x_s)] - \sum_{s=1}^{n_0} \sin(jx_s^*) J_{0,s}^* \right)$$

$$+ \frac{1}{\pi j} \sum_{s=1}^{n_1} \cos(jx_s) \left[ f'(x_s) \right] + O\left( j^{-2} \right),$$

as $j \to \infty$. Here $n_1$ is the (unknown) number of points of discontinuity in $f'$. (We shall assume that $n_1 \geq n_0$, by including all of the points of simple discontinuity of $f$ in the set of points where $f'$ may be discontinuous.) Using Eqs.(11), we write Eqs.(4.3) as

$$a_j^{(1)} = \frac{1}{\pi} \sum_{s=1}^{n_0} [f'(x_s)] \left( \frac{j}{N^2} - \frac{1}{j} \right) \sin(jx_s) + O\left( \frac{1}{N^2} \right)$$

$$- \frac{1}{\pi j} \sum_{s=n_0+1}^{n_1} [f'(x_s)] \sin(jx_s) + O\left( j^{-2} \right),$$

(4.4)
$$b_j^{(1)} = \frac{1}{\pi} \sum_{s=1}^{n_0} [f'(x_s)] \left( \frac{1}{j} - \frac{j}{N^2} \right) \cos(jx_s) + O\left( \frac{1}{N^2} \right)$$

$$+ \frac{1}{\pi j} \sum_{s=n_0+1}^{n_1} [f'(x_s)] \cos(jx_s) + O\left( j^{-2} \right),$$

as $j \to \infty$. (Here the points $\{x_s\}$, $s = n_0 + 1, ..., n_1$, correspond to contact singularities of $f$ of order one.)

We now make two observations. First, by comparing Eqs.(4.4) and Eqs.(3.1), we see that, for $x$ near the contact singularity at $x_s$, $s = n_0 + 1, ..., n_1$, the partial sums $\{F_{1,N}\}$ behave like a function which has a *simple discontinuity* at this point of magnitude $[f'(x_s)]$. Thus, if we define a new partial sum $D_{1,N}(x)$ as in Eq.(2.2), but based on the partial sum $F_{1,N}$, instead of $F_N$, i.e.,

(4.5)
$$D_{1,N}(x) = \frac{F_{1,N}(x + \pi/(N+1)) - F_{1,N}(x - \pi/(N+1))}{(2/\pi)\operatorname{Si}(\pi)},$$

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then it follows that

$$D_{1,N}(x_s) \to [f'(x_s)], \quad \text{at a point of } contact \text{ discontinuity,}$$

as $N \to \infty$. Second, to investigate the behavior of $D_{1,N}(x)$ near the point of simple discontinuity at $x_s$, $s = 1, 2, ..., n_0$, we first observe (following the same reasoning as in Carslaw [2]) that

$$\lim_{N \to \infty} F_{1,N}\left(\eta_{s,\pm}\right) = \frac{f'(x_s^+) + f'(x_s^-)}{2} \pm \frac{1}{\pi}\left(\text{Si}(\pi) - \frac{1}{\pi}\right)[f'(x_s)].$$

Thus, it follows that

$$D_{1,N}(x_s) \to \left(\frac{\text{Si}(\pi) - 1/\pi}{\text{Si}(\pi)}\right)[f'(x_s)], \quad \text{at a point of } simple \text{ discontinuity,}$$

as $N \to \infty$. (Here $(\text{Si}(\pi) - 1/\pi)/\text{Si}(\pi) \doteq 0.82812$.) For any point $x$ that is *not* a point of simple discontinuity or contact discontinuity of $f$, $D_{1,N}(x) \to 0$, as $N \to \infty$.

To illustrate these ideas, we use them to find initial estimates of points of first order singularity of $f$ for Example 1. In Fig.5, we have plotted $D_{1,N}$ for this example with several values of $N$. The absolute errors in the estimate of the point of contact discontinuity at $x_2 = 1$, and the relative errors in the estimation of the associated jump $[f'(1)]$, using the partial sums of $D_{1,N}$, are summarized in Table 6 for several values of $N$. The relative errors in the estimation of the jump $[f'(3)]$ are also listed. Similar to the method of Section 2, we can show, in general, that, using the partial sums $\{D_{1,N}\}$, the error in approximating the locations of the points of contact discontinuities is $O(N^{-2})$, while the error in the approximations to all of the jumps $[f'(x_s)]$ is $O(N^{-1})$.

| $N$ | Abs. Error in $\tilde{x}_2$ | Rel. Error in $D_{1,N}(\tilde{x}_2)]$ | Rel. Error in $D_{1,N}(\tilde{x}_1)]$ |
|---|---|---|---|
| 16 | $2.1 \cdot 10^{-3}$ | $7.4 \cdot 10^{-3}$ | $4.5 \cdot 10^{-1}$ |
| 32 | $2.4 \cdot 10^{-5}$ | $1.5 \cdot 10^{-3}$ | $2.2 \cdot 10^{-1}$ |
| 64 | $1.2 \cdot 10^{-5}$ | $7.8 \cdot 10^{-5}$ | $1.1 \cdot 10^{-1}$ |
| 128 | $5.4 \cdot 10^{-7}$ | $2.0 \cdot 10^{-6}$ | $5.1 \cdot 10^{-2}$ |
| 256 | $2.7 \cdot 10^{-8}$ | $2.9 \cdot 10^{-6}$ | $2.5 \cdot 10^{-2}$ |

**Table 6:** Errors in the initial estimates of the discontinuities in $f'$ for Example 1 using the partial sums $\{D_{1,N}\}$.

**5. Discontinuities in $f'(x)$ - improved estimates.** Once the number of discontinuities in $f$ and $f'$ are determined, as well as initial estimates of the locations and magnitudes of all of the jumps in $f$ and $f'$, we again seek to improve these estimates by using a least-squares fit of the asymptotic form of the coefficients to the given coefficients. Using Lemma 3.1 with $M = 1$, we now define

$$(5.1) \qquad E = E\left(\hat{x}_1, ..., \hat{x}_{n_1}, \hat{J}_{0,1}, ..., \hat{J}_{0,n_1}, \hat{J}_{1,1}, ..., \hat{J}_{1,n_1}\right) \equiv \sum_{j=N+1-R}^{N} \omega_j E_j^{(1)},$$

where

$$E_j^{(1)} \equiv \left(j^2 \pi a_j + \sum_{s=1}^{n_1} \left\{j \sin(j\hat{x}_s)\hat{J}_{0,s} + \cos(j\hat{x}_s)\hat{J}_{1,s}\right\}\right)^2 +$$

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$$(5.2) \qquad \left( j^2 \pi b_j - \sum_{s=1}^{n_1} \left\{ j \cos(j\hat{x}_s)\hat{J}_{0,s} - \sin(j\hat{x}_s)\hat{J}_{1,s} \right\} \right)^2 .$$

(Note that, for ease of notation, we have let the index $s$ range up to $n_1$, with the understanding that $\hat{J}_{0,s} \equiv 0$, for $s = n_0+1, ..., n_1$.) Then, given the coefficients $\{a_j, b_j\}$, we seek to determine the values of $\left\{ \hat{x}_s, \hat{J}_{0,s}, \hat{J}_{1,s} \right\}$, say $\left\{ x_s^*, J_{0,s}^*, J_{1,s}^* \right\}$, $s = 1, 2, ..., n_1$, such that $E$ is a *minimum*, i.e.,

$$(5.3) \qquad \min_{\hat{x}_s, \hat{J}_{0,s}, \hat{J}_{1,s}} E\left( \hat{x}_1, ..., \hat{J}_{0,1}, ..., \hat{J}_{1,n_1} \right) = E\left( x_1^*, ..., J_{0,1}^*, ..., J_{1,n_1}^* \right) .$$

(Since there are now $3n_1$ parameters to be estimated, we require $R \geq 3n_1/2$.)

From Eqs.(5.1)-(5.3), it follows, for the case when $\omega_j = 1$, that

$$x_s^* = x_s + O\left( 1/N^5 \right), \quad 1 \leq s \leq n_0,$$

$$x_s^* = x_s + O\left( 1/N^3 \right), \quad n_0 + 1 \leq s \leq n_1,$$

$$(5.4) \qquad J_{0,s}^* = [f(x_s)] - [f''(x_s)]\frac{1}{N^2} + O(1/N^3), \quad 1 \leq s \leq n_0,$$

$$J_{1,s}^* = [f'(x_s)] + O\left( 1/N^2 \right), \quad 1 \leq s \leq n_1,$$

as $N \to \infty$.

In Table 7, the absolute error in estimating the point of contact discontinuity at $x_2 = 1$ for Example 1, and the relative errors in the estimation of the jumps $[f'(1)]$ and $[f'(3)]$, using the method just described, are summarized.

| $N$ $(R)$ | $x_2^*$ | $J_{1,2}^*$ | $x_1^*$ | $J_{0,1}^*$ | $J_{1,1}^*$ |
|---|---|---|---|---|---|
| 32 (15) | $2.1 \cdot 10^{-4}$ | $1.47 \cdot 10^{-2}$ | $3.29 \cdot 10^{-5}$ | $4.16 \cdot 10^{-3}$ | $1.97 \cdot 10^{-2}$ |
| 64 (18) | $8.14 \cdot 10^{-5}$ | $2.0 \cdot 10^{-3}$ | $1.95 \cdot 10^{-6}$ | $1.00 \cdot 10^{-3}$ | $2.72 \cdot 10^{-3}$ |
| 128 (20) | $1.93 \cdot 10^{-6}$ | $7.19 \cdot 10^{-4}$ | $7.24 \cdot 10^{-7}$ | $2.41 \cdot 10^{-4}$ | $3.17 \cdot 10^{-3}$ |
| 256 (46) | $6.4 \cdot 10^{-7}$ | $1.56 \cdot 10^{-4}$ | $2.00 \cdot 10^{-9}$ | $6.41 \cdot 10^{-5}$ | $2.17 \cdot 10^{-4}$ |

**Table 7:** Errors in the estimates of the discontinuities in $f$ and $f'$ for Example 1 using the LSPE method with $M = 1$.

Comparing Table 7 to Table 6 illustrates that the errors in the estimates of $[f'(x_1)]$ are significantly smaller using the least-squares approach. Of course, we also obtain "new" estimates of the location and magnitude of the discontinuity in $f$ at $x_1 = 3$. The corresponding errors are also shown in Table 7. We observe that the errors in the estimates of $[f'(x_2)]$, and the location of the first order contact discontinuity (at $x_2 = 1$) are somewhat greater when compared with the errors in the initial estimates they use. This should not, however, be a cause of concern, as the estimates that are obtained using the LSPE method are *good*, and are within the order of accuracy that is predicted for them (see Eqs.(5.4)).

**6. Estimation of discontinuities of order $M$, for $M \geq 2$.** Assume now that we have used the methods of the previous sections and that we have obtained, by the LSPE method, estimates $\{x_s^*\}$ and $\left\{ J_{k,s}^* \right\}$ of the locations $\{x_s\}$ and the associated jumps $\left[ f^{(k)}(x_s) \right]$, respectively, of the singularities of $f$, for

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$k = 0, 1, ..., M - 1$, and $s = 1, 2, ..., n_{M-1}$. We define

$$a_j^{(M-1)} = a_j - \frac{1}{\pi} \left\{ \sum_{s=1}^{n_{M-1}} \sin(jx_s^*) \left( \sum_{k=0}^{\lfloor (M-1)/2 \rfloor} \frac{(-1)^{k+1}}{j^{2k+1}} J_{2k,s}^* \right) \right.$$

$$\left. + \cos(jx_s^*) \left( \sum_{k=0}^{\lfloor (M-2)/2 \rfloor} \frac{(-1)^{k+1}}{j^{2k+2}} J_{2k+1,s}^* \right) \right\}$$

$$b_j^{(M-1)} = b_j - \frac{1}{\pi} \sum_{s=1}^{n_{M-1}} \left\{ \cos(jx_s^*) \left( \sum_{k=0}^{\lfloor (M-1)/2 \rfloor} \frac{(-1)^{k}}{j^{2k+1}} J_{2k,s}^* \right) \right.$$

$$\left. + \sin(jx_s^*) \left( \sum_{k=0}^{\lfloor (M-2)/2 \rfloor} \frac{(-1)^{k+1}}{j^{2k+2}} J_{2k+1,s}^* \right) \right\},$$

and the partial sums

$$F_{M,N}(x) = \left( \frac{d}{dx} \right)^M \sum_{j=1}^N \left\{ a_j^{(M-1)} \cos(jx) + b_j^{(M-1)} \sin(jx) \right\}$$

$$= \sum_{j=1}^N \left\{ a_j^{(M)} \cos(jx) + b_j^{(M)} \sin(jx) \right\},$$

where

$$a_j^{(M)} \equiv (-1)^{\lfloor M/2 \rfloor} j^M a_j^{(M-1)}, \quad b_j^{(M)} \equiv (-1)^{\lfloor M/2 \rfloor} j^M b_j^{(M-1)}, \quad M \text{ even,}$$

$$a_j^{(M)} \equiv (-1)^{\lfloor M/2 \rfloor} j^M b_j^{(M-1)}, \quad b_j^{(M)} \equiv -(-1)^{\lfloor M/2 \rfloor} j^M a_j^{(M-1)}, \quad M \text{ odd.}$$

Here, in general, $n_j$ denotes the number of points in the interval $(-\pi, \pi]$ where $f^{(k)}$ has a discontinuity for at least one value of $k \le j$.

To find initial estimates of the locations and magnitudes of the discontinuities in $f^{(M)}$, we define

$$D_{M,N}(x) = \frac{F_{M,N}(x + \pi/(N+1)) - F_{M,N}(x - \pi/(N+1))}{(2/\pi)\,\text{Si}(\pi)}.$$

Then it follows that

$$D_{M,N}(x_s) \rightarrow \begin{cases} \alpha_{M,s} \cdot \left[ f^{(M)}(x_s) \right], & s = 1, 2, ..., n_M, \\ 0, & \text{otherwise,} \end{cases}$$

as $N \to \infty$. Here $\alpha_{M,s}$ is a scalar that depends on both $M$ and $s$. In particular,

$$\alpha_{2,s} = \begin{cases} (\text{Si}(\pi) - 1/\pi)/\text{Si}(\pi), & 1 \le s \le n_0, \\ 1, & n_0 + 1 \le s \le n_2, \end{cases}$$

and

$$\alpha_{3,s} = \begin{cases} (\text{Si}(\pi) - 1/\pi - 6/\pi^3)/\text{Si}(\pi), & 1 \le s \le n_0, \\ (\text{Si}(\pi) - 2/\pi)/\text{Si}(\pi), & n_0 + 1 \le s \le n_1, \\ 1, & n_1 + 1 \le s \le n_3. \end{cases}$$

Thus, $D_{M,N}(x)$ can be used to find initial estimates of the locations and magnitudes of the jumps in $f^{(M)}(x)$, as in Sections 2 and 4.

To illustrate these ideas, we set $M = 2$ and use $D_{2,N}(x)$ to estimate the locations and magnitudes of the jumps in $f''$ for Example 1. The results are summarized in Table 8. (We find that $D_{2,N}(x) \to 0$ in a neighborhood of $x = x_2 = 1$, suggesting that $[f''(x_2)]$ is zero.)

| $N$ | Abs. Error in $D_{2,N}(\tilde{x}_2)$ | Abs. Error in $\tilde{x}_3$ | Rel. Error in $D_{2,N}(\tilde{x}_3)$ |
|---|---|---|---|
| 32 | $2.57 \cdot 10^{-1}$ | $1.94 \cdot 10^{-3}$ | $3.07 \times 10^{-2}$ |
| 64 | $1.03 \cdot 10^{-1}$ | $5.07 \times 10^{-4}$ | $1.53 \times 10^{-2}$ |
| 128 | $3.49 \cdot 10^{-1}$ | $1.33 \times 10^{-4}$ | $7.73 \times 10^{-3}$ |
| 256 | $3.03 \cdot 10^{-1}$ | $3.30 \cdot 10^{-5}$ | $3.89 \cdot 10^{-3}$ |

**Table 8:** Errors in the initial estimate of the discontinuities in $f''$ for Example 1 using the partial sums $\{D_{2,N}\}$.

Once initial estimates of the locations and magnitudes of the jumps in $f^{(M)}$ have been determined, we again improve these estimates by using a least-squares fit to the asymptotic form of the coefficients. Thus, we define

$$(6.1) \qquad E \equiv \sum_{j=N-R+1}^{N} \omega_j E_j^{(M)},$$

$$(6.2) \qquad E_j^{(M)} \equiv \left( j^{M+1} \pi a_j - \sum_{s=1}^{n_M} \left[ \sin(j\hat{x}_s) \left\{ \sum_{k=0}^{[M/2]} (-1)^{k+1} j^{M-2k} \hat{J}_{2k,s} \right\} + \right.\right.$$
$$\left.\left. \cos(j\hat{x}_s) \left\{ \sum_{k=0}^{[(M-1)/2]} (-1)^{k+1} j^{M-1-2k} \hat{J}_{2k+1,s} \right\} \right] \right)^2 +$$
$$\left( j^{M+1} \pi b_j - \sum_{s=1}^{n_M} \left[ \cos(j\hat{x}_s) \left\{ \sum_{k=0}^{[M/2]} (-1)^k j^{M-2k} \hat{J}_{2k,s} \right\} + \right.\right.$$
$$\left.\left. \sin(j\hat{x}_s) \left\{ \sum_{k=0}^{[(M-1)2]} (-1)^{k+1} j^{M-1-2k} \hat{J}_{2k+1,s} \right\} \right] \right)^2,$$

and choose values of the $n_M(2+M)$ parameters $\{\hat{x}_s\}$ and $\left\{ \hat{J}_{k,s} \right\}$, say, $\left\{ x_s^*, J_{k,s}^* \right\}$, $s = 1, 2, ..., n_M$, $k = 0, 1, ..., M$, so that $E$ is a *minimum*, i.e.,

$$\min_{\hat{x}_s, ..., \hat{J}_{k,s}} E\left( \hat{x}_1, ..., \hat{J}_{0,1}, ..., \hat{J}_{M,n_M} \right) = E\left( x_1^*, ..., J_{0,1}^*, ..., J_{M,n_M}^* \right).$$

Here $R \geq n_M(2+M)/2$, with $N - R \gg 1$.

When we apply these ideas to Example 1 with $M = 2$, we obtain the results whose errors are summarized in Tables 9 and 10. (We find that the estimates obtained for $[f''(x_2)]$ suggest, rightfully, that $[f''(x_2)] = 0$.)

Setting $M = 3$, we find initial and improved estimates of the contact singularity of order 3 at $x_4 = 5$ for Example 1. In this case, the maximum error for the location or associated jump in any of the improved estimates is of the order of $10^{-13}$. To understand why the errors should be so small, we note that, since $f$

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of Example 1 is piece-wise polynomial, of degree at most 3, the assumed form of the Fourier coefficients in Eq.(6.2) is exact for $M \geq 3$. Hence, the estimates obtained by the method are "essentially exact", to within the error inherent in the minimization procedure.

| $N$ $(R)$ | $x_1^*$ | $J_{0,1}^*$ | $J_{1,1}^*$ | $J_{2,1}^*$ |
|---|---|---|---|---|
| 32(18) | $1.83 \cdot 10^{-6}$ | $2.92 \cdot 10^{-5}$ | $5.33 \cdot 10^{-4}$ | $5.4 \cdot 10^{-3}$ |
| 64(22) | $6.3 \cdot 10^{-8}$ | $1.33 \cdot 10^{-6}$ | $1.03 \cdot 10^{-4}$ | $3.22 \cdot 10^{-3}$ |
| 128(32) | $1.0 \cdot 10^{-9}$ | $1.03 \cdot 10^{-7}$ | $5.67 \cdot 10^{-6}$ | $9.8 \cdot 10^{-4}$ |
| 256(56) | $8.75 \cdot 10^{-11}$ | $2.73 \cdot 10^{-8}$ | $1.67 \cdot 10^{-6}$ | $4.5 \cdot 10^{-4}$ |

**Table 9:** Errors in the estimates of the discontinuity at $x_1 = 3$ and the associated jumps for Example 1 using the LSPE method with $M = 2$.

| $N$ $(R)$ | $x_2^*$ | $J_{1,2}^*$ | $J_{2,2}^*$ | $x_3^*$ | $J_{2,3}^*$ |
|---|---|---|---|---|---|
| 32(18) | $3.95 \cdot 10^{-5}$ | $5.72 \cdot 10^{-4}$ | $2.3 \cdot 10^{-2}$ | $5.4 \cdot 10^{-4}$ | $7.75 \cdot 10^{-4}$ |
| 64(22) | $3.0 \cdot 10^{-6}$ | $8.09 \cdot 10^{-6}$ | $9.1 \cdot 10^{-3}$ | $1.14 \cdot 10^{-4}$ | $1.99 \cdot 10^{-4}$ |
| 128(32) | $5.0 \cdot 10^{-7}$ | $2.8 \cdot 10^{-6}$ | $6.67 \cdot 10^{-3}$ | $2.9 \cdot 10^{-5}$ | $1.25 \cdot 10^{-4}$ |
| 256(56) | $1.96 \cdot 10^{-8}$ | $1.5 \cdot 10^{-6}$ | $1.43 \cdot 10^{-3}$ | $7.06 \cdot 10^{-6}$ | $1.24 \cdot 10^{-5}$ |

**Table 10:** Errors in the estimates of the discontinuities at $x_2 = 1$ and $x_3 = 4$, and the associated jumps, for Example 1 using the LSPE method with $M = 2$.

| $N(R)$ | $x_1^*$ | $J_{0,1}^*$ | $J_{1,1}^*$ |
|---|---|---|---|
| 32(15) | $3.29 \cdot 10^{-5}$ | $1.55 \cdot 10^{-3}$ | $2.44 \cdot 10^{-2}$ |
| 64(18) | $1.17 \cdot 10^{-6}$ | $3.49 \cdot 10^{-4}$ | $3.28 \cdot 10^{-3}$ |
| 128(24) | $1.65 \cdot 10^{-8}$ | $7.35 \cdot 10^{-5}$ | $2.65 \cdot 10^{-4}$ |
| 256(41) | $2.15 \cdot 10^{-9}$ | $1.77 \cdot 10^{-5}$ | $1.63 \cdot 10^{-4}$ |

**Table 11:** Errors in the estimates of the discontinuity at $x_1 = 1$ for Example 2 using the LSPE method with $M = 1$.

On applying the above mentioned ideas to Example 2 with $M = 1$ and $M = 2$, we obtain results that are qualitatively similar to those for Example 1. The results for the discontinuity at $x_1 = 1$ are summarized in Tables 11 and 12. The results for the other points of discontinuity in $f$ are qualitatively similar to those reported in Tables 11 and 12.

| $N(R)$ | $x_1^*$ | $J_{0,1}^*$ | $J_{1,1}^*$ | $J_{2,1}^*$ |
|---|---|---|---|---|
| 32(15) | $2.96 \cdot 10^{-6}$ | $1.29 \cdot 10^{-5}$ | $3.54 \cdot 10^{-3}$ | $1.38 \cdot 10^{-2}$ |
| 64(22) | $1.28 \cdot 10^{-7}$ | $8.29 \cdot 10^{-7}$ | $7.29 \cdot 10^{-4}$ | $3.34 \cdot 10^{-3}$ |
| 128(32) | $6.47 \cdot 10^{-9}$ | $2.26 \cdot 10^{-8}$ | $1.63 \cdot 10^{-4}$ | $3.94 \cdot 10^{-4}$ |
| 256(60) | $3.72 \cdot 10^{-10}$ | $2.92 \cdot 10^{-9}$ | $3.91 \cdot 10^{-5}$ | $1.16 \cdot 10^{-4}$ |

**Table 12:** Errors in the estimates of the discontinuity at $x_1 = 1$ for Example 2 using the LSPE method with $M = 2$.

For a general value of $M \geq 0$, we conjecture that the estimates obtained from the LSPE method satisfy

$$(6.3) \qquad x_s^* = x_s + O(N^{-M-2}), \quad s = 1, 2, ..., n,$$

and

$$(6.4) \qquad J_{k,s}^* = \left[ f^{(k)}(x_s) \right] + O(N^{-M-1+k}), \quad k = 0, 1, ..., M, \quad s = 1, 2, ..., n.$$

Although we do not have an analytical proof of these results, they have been verified using Mathematica [22] for $0 \leq M \leq 4$ and for $1 \leq n \leq 6$. Also, the results of several numerical experiments are consistent with them.

**7. Comparison with other methods.** Three recent methods with a similar goal of obtaining estimates of the locations of the discontinuities of $f$ from a finite number of its Fourier coefficients have been proposed by Eckhoff [3], Kvernadze [15], and Bauer [1].

Eckhoff [3] develops an algebraic equation of degree $n$ for the $n$ singularity locations in each period of $f$. The coefficients in his equation are obtained by solving an algebraic system of $n$ equations, determined by the known coefficients in the truncated Fourier series. If discontinuities in the derivatives of $f$ are considered, in addition to the simple discontinuities of $f$, that algebraic system is *nonlinear* in the unknown parameters. The degree of the algebraic system depends on the desired order $M$ for the reconstruction, with a higher value of $M$ normally leading to a more accurate determination of the singularity locations. The jumps in $f$ and its derivatives, up to the order $M$, can be obtained by solving an additional linear algebraic system of equations. However, the robustness of the method deteriorates with increasing values of $M$. This is due to the ill-conditioned nature of the equations that must be solved.

Kvernadze [15] proposes an algorithm to determine the discontinuities and the corresponding jumps in $f$ using certain identities based on the partial sums of its differentiated Fourier series. Kvernadze first analyzes an expansion formula for the approximation of a $2\pi$-periodic, piecewise smooth function with one discontinuity. An appropriate linear combination of certain identities, obtained via derivatives of different orders, is then used to significantly improve the accuracy of the estimation. It is then suggested that Richardson's extrapolation method be used to refine the accuracy even further. For a function with multiple discontinuities, Kvernadze establishes a formula that *eliminates* all but one discontinuity in the function, and then treats the new function as one with a single point of discontinuity. Kvernadze does not address aspects of the numerical complexity and robustness of his algorithm.

Bauer [1] uses the idea of band pass filters to find the discontinuity locations. He makes no effort to estimate the associated jumps or the points of contact discontinuities. In his work, Bauer introduces the idea of a global filter and a local sub-cell filter. There is a trade off between these two filters. Smaller errors can be obtained using a local sub-cell filter, but the accuracy decreases if there is a contact discontinuity. His global filter can be computed "once" and stored in memory, but the local filer cannot be computed until initial estimates of the locations of the discontinuities are determined. A comparison of Eckhoff's, Kvernadze's, and Bauer's methods show that, for a given value of $N$, Eckhoff's results are consistently more accurate and robust. Also, Bauer's local-filter method appears to be unable to control the error if the function has a contact discontinuity.

The LSPE method we are proposing is based on a simple idea, is remarkably robust (see the next section), and requires only "standard" optimization techniques to implement. The method appears to provide estimates of the discontinuity locations which are of the same order of accuracy (or better) than those of Eckhoff, Kvernadze, and Bauer. In addition, the LSPE method provides estimates (of high accuracy) of the associated jumps in $f$ and its derivatives at the points of discontinuity.

To illustrate this comparison, the function $f$ of our Example 2 was also considered by Eckhoff, Kvernadze, and Bauer. The absolute value of the *largest* error in the estimation of the points of simple discontinuity of $f$, obtained by Bauer, by Eckhoff, by Kvernadze, and by the LSPE method are summarized in Tables 13-16, for different values of $N$ and $M$.

| $N$ | 32 | 64 | 128 | 256 |
|---|---|---|---|---|
| Local Filter | $1.4 \cdot 10^{-5}$ | $1.44 \cdot 10^{-6}$ | $5.62 \cdot 10^{-9}$ | $3.14 \cdot 10^{-9}$ |
| Global Filter | $1.5 \cdot 10^{-3}$ | $8.77 \cdot 10^{-5}$ | $2.26 \cdot 10^{-6}$ | $2.71 \cdot 10^{-7}$ |

Table 13: Maximum errors in the estimates of the singularity locations for Example 2 using Bauer's method.

| $N$ | 32 | 64 | 128 | 256 |
|---|---|---|---|---|
| $M = 0$ | $1.4 \cdot 10^{-3}$ | $3.1 \cdot 10^{-4}$ | $7.3 \cdot 10^{-5}$ | $1.8 \cdot 10^{-5}$ |
| $M = 1$ | $2.2 \cdot 10^{-5}$ | $1.0 \cdot 10^{-6}$ | $5.6 \cdot 10^{-8}$ | $2.7 \cdot 10^{-9}$ |
| $M = 2$ | $4.0 \cdot 10^{-6}$ | $1.2 \cdot 10^{-7}$ | $5.1 \cdot 10^{-9}$ | $2.7 \cdot 10^{-10}$ |
| $M = 3$ | $1.2 \cdot 10^{-7}$ | $2.8 \cdot 10^{-10}$ | $5.3 \cdot 10^{-11}$ | $4.4 \cdot 10^{-5}$ |

Table 14: Maximum errors in the estimates of the singularity locations for Example 2 using Eckhoff's method.

Tables 13-16 illustrate the convergence of all the methods. The results obtained by Eckhoff's method and the LSPE method are generally more accurate (for $M \geq 2$) than Bauer's results and Kvernadze's results. The robustness of Eckhoff's method deteriorates when $M \geq 3$. This pattern becomes evident on comparison of results of his method to our results when $M = 3$. We find that for larger values for $N$, Eckhoff's method deteriorates significantly, while the LSPE method appears to show no such adverse effect.

| $N$ | 32 | 64 | 128 | 256 |
|---|---|---|---|---|
| Kvernadze | $1.7 \cdot 10^{-4}$ | $6.1 \cdot 10^{-7}$ | $1.4 \cdot 10^{-8}$ | $3.5 \cdot 10^{-11}$ |

Table 15: Maximum errors in the estimates of the singularity locations for Example 2 using Kvernadze's method.

| $N$ | 32 | 64 | 128 | 256 |
|---|---|---|---|---|
| $M = 0$ | $1.59 \cdot 10^{-3}$ | $3.31 \cdot 10^{-4}$ | $7.73 \cdot 10^{-5}$ | $1.78 \cdot 10^{-5}$ |
| $M = 1$ | $1.45 \cdot 10^{-4}$ | $1.17 \cdot 10^{-6}$ | $2.17 \cdot 10^{-7}$ | $1.44 \cdot 10^{-8}$ |
| $M = 2$ | $2.95 \cdot 10^{-6}$ | $1.38 \cdot 10^{-7}$ | $7.1 \cdot 10^{-9}$ | $4.26 \cdot 10^{-10}$ |
| $M = 3$ | $6.86 \cdot 10^{-8}$ | $4.14 \cdot 10^{-9}$ | $4.9 \cdot 10^{-11}$ | $1.47 \cdot 10^{-13}$ |

Table 16: Maximum errors in the estimates of the singularity locations for Example 2 using the LSPE method.

**8. Robustness of the LSPE method.** Intuitively, the LSPE method should possess good robustness characteristics, due primarily to the underlying least-squares nature of the method and the fact that the objective function is an "average" involving several Fourier coefficients. Although we have not carried out a detailed analysis of the robustness of the LSPE method, in this section we consider some of its robustness properties suggested by three more examples.

**Example 3.** We consider again the function of Example 2, but we now contaminate its Fourier coefficients by introducing some *random errors*. We then apply the LSPE method using these contaminated coefficients, and compare the results with those obtained using the original ("exact") coefficients. Letting $\{a_j, b_j\}$ denote the exact Fourier coefficients of $f$, we define the new coefficients

$$\tilde{a}_j = a_j + \epsilon_{a,j}, \quad \tilde{b}_j = b_j + \epsilon_{b,j}, \quad 1 \leq j \leq N,$$

where $\epsilon_{a,j}$ and $\epsilon_{b,j}$ are independent, uniformly distributed random variables on the interval $[-\epsilon, \epsilon]$, with $\epsilon > 0$ specified.

The relative errors in the estimates of $x_1 = 1$, as well as the corresponding jump in $f$, using the LSPE method with $M = 0$, $N = 64$, and $R = 32$, are summarized in Table 17, for a range of values of $\epsilon$. The estimates of $x_1$ and $[f(x_1)]$ appear to improve only marginally with decreasing values of $\epsilon$ in the range considered.

| $\epsilon$ | $x_1^*$ | $J_{0,1}^*$ |
|---|---|---|
| $10^{-2}$ | $1.48 \cdot 10^{-3}$ | $4.0 \cdot 10^{-2}$ |
| $10^{-3}$ | $2.0 \cdot 10^{-4}$ | $3.723 \cdot 10^{-3}$ |
| $10^{-4}$ | $3.73 \cdot 10^{-4}$ | $5.27 \cdot 10^{-4}$ |
| $0$ | $3.92 \cdot 10^{-4}$ | $1.77 \cdot 10^{-4}$ |

**Table 17:** Errors in the estimates of the location and the magnitude of the discontinuity at $x_1 = 1$ for Example 3 using contaminated coefficients in the LSPE method with $M = 0$.

Results for the case $M = 1$, $N = 64$, and $R = 32$, are summarized in Table 18. The estimates of $x_1$ and $[f(x_1)]$ appear to be relatively insensitive to the increase in the order for $M$, for the range of values of $\epsilon$ considered. However, there is a noticeable improvement in the estimates of $[f'(x_1)]$ with decreasing $\epsilon$. This sensitivity of the higher order jump estimates to $\epsilon$ is explained by considering the form of Eq.(5.1) that is used for the least-squares parameter estimation. The effect of a multiplier that is a power of $j$ is likely to have an adverse effect on parameters that are dependent on higher precision digits in the Fourier coefficients. As a result, we see a noticeable increase in the accuracy of the estimate of $[f'(x_1)]$ with decreasing values of $\epsilon$. (Errors for the other singularities of $f$ are comparable to those in Tables 17 and 18.)

| $\epsilon$ | $x_1^*$ | $J_{0,1}^*$ | $J_{1,1}^*$ |
|---|---|---|---|
| $10^{-2}$ | $7.52 \cdot 10^{-3}$ | $1.03 \cdot 10^{-2}$ | $12.31$ |
| $10^{-3}$ | $6.82 \cdot 10^{-4}$ | $1.53 \cdot 10^{-3}$ | $0.97$ |
| $10^{-4}$ | $6.92 \cdot 10^{-5}$ | $2.05 \cdot 10^{-4}$ | $0.1$ |
| $10^{-5}$ | $8.69 \cdot 10^{-6}$ | $3.72 \cdot 10^{-4}$ | $1.49 \cdot 10^{-2}$ |
| $0$ | $1.97 \cdot 10^{-6}$ | $3.97 \cdot 10^{-4}$ | $5.51 \cdot 10^{-3}$ |

**Table 18:** Errors in the estimates of the discontinuity location and the associated jumps for Example 3 using contaminated coefficients in the LSPE method with $M = 1$.

**Example 4.** To help assess the effect of the *closeness of two points of discontinuity* on the computed results, for $0 < a < 2\pi - 1$ we define

$$(8.1) \qquad f(x) = \begin{cases} x, & 1 < x < 1 + a \\ 0, & \text{elsewhere in } [0, 2\pi] \end{cases}, \quad f(x + 2\pi) = f(x).$$

For this example $f$ has discontinuities at $x_1 = 1$ and at $x_2 = 1 + a$. The relative errors in the estimates of $x_1$ and $x_2$, as well as the corresponding jumps in $f$, using the LSPE method with $M = 0$, $N = 64$ and $R = 15$, are summarized in Table 19, for a range of values of $a$. All of the estimates of the parameters shown appear to be relatively insensitive to the value of $a$ in the range considered. Results obtained by Bauer's method, on the other hand, appear to be significantly more sensitive to the distance between two consecutive singularities, especially as $a \to 0$.

| $a$ | $x_1^*$ | $J_{1,0}^*$ | $x_2^*$ | $J_{2,0}^*$ |
|-----|---------|-------------|---------|-------------|
| 0.1 | $3.8 \cdot 10^{-4}$ | $6.89 \cdot 10^{-4}$ | $3.14 \cdot 10^{-4}$ | $2.97 \cdot 10^{-4}$ |
| 0.5 | $3.1 \cdot 10^{-4}$ | $6.46 \cdot 10^{-4}$ | $1.38 \cdot 10^{-4}$ | $2.58 \cdot 10^{-4}$ |
| 0.9 | $3.09 \cdot 10^{-4}$ | $3.68 \cdot 10^{-4}$ | $8.57 \cdot 10^{-5}$ | $6.94 \cdot 10^{-5}$ |
| 2.0 | $3.03 \cdot 10^{-4}$ | $1.91 \cdot 10^{-4}$ | $3.37 \cdot 10^{-5}$ | $1.31 \cdot 10^{-4}$ |

**Table 19:** Errors in the estimates of the location and magnitude of the discontinuities for Example 4 for a range of values of $a$ using the LSPE method with $M = 0$.

**Example 5.** We now illustrate some of the robustness of the LSPE method with respect to *noise in sampled data.* In this case, the Fourier coefficients of a function $f$ are computed using a Fast Fourier Transform (FFT) method applied to a data set of (slightly erroneous) functional values at evenly spaced values of the independent variable.

We define $f$ as the "usual" step function, but with small random errors, as

$$(8.2) \qquad f(x) = \begin{cases} -1 + \epsilon_1, & 0 < x < \pi, \\ 1 + \epsilon_2, & \pi < x < 2\pi, \end{cases} \qquad f(x + 2\pi) = f(x).$$

Here $\epsilon_1$ and $\epsilon_2$ are independent random variables that are uniformly distributed over the interval $[-\epsilon, \epsilon]$, with $\epsilon > 0$ specified. Then $f$ has two simple discontinuities, at $x_1 = \pi$ and at $x_2 = 2\pi$. We observe that there are two major sources of error in the computed Fourier coefficients. One source of error is the noise amplitude $\epsilon$, which is introduced into $f$ and, hence, into the sampled functional values. Another source of error is the use of the FFT, which uses only a finite number of sample points. For example, using $2N + 1$ sample points, only the first $2N + 1$ Fourier coefficients can be estimated, before aliasing occurs (see, e.g., Hamming [13]). When error is introduced into the data, it is natural to expect the relative error in the computed Fourier coefficients to increase with increasing index. As a result, instead of using the *last* $R$ coefficients, we find that it is better to base the LSPE method on some of the lower order coefficients. For our illustration, we used a sample of size 65 (from which we can estimate the first 32 $\{a_j\}$ and $\{b_j\}$), but we only use the ninth through the fifteenth coefficients in the definition of $E$. The relative errors in the estimates of $x_1$ and $[f(x_1)]$ using the LSPE method, with $M = 0$, are summarized in Table 20.

| $N = 15, R = 7$ | Abs. Error in $x_1^*$ | Rel. Error in $J_{0,1}^*$ |
|-----------------|----------------------|---------------------------|
| Exact, $\epsilon = 0$ | $1.0 \cdot 10^{-17}$ | $1.0 \cdot 10^{-17}$ |
| $FFT, \epsilon = 0$ | $1.33 \cdot 10^{-2}$ | $5.5 \cdot 10^{-3}$ |
| $FFT, \epsilon = 10^{-2}$ | $1.28 \cdot 10^{-2}$ | $7.5 \cdot 10^{-3}$ |

**Table 20:** Errors in the estimates of the location and the magnitude of the discontinuity for Example 5 using the LSPE method with $M = 0$. The Fourier coefficients are computed from complete and sampled data.

From Table 20, we note that there is virtually no error if the *exact* Fourier coefficients ($\epsilon = 0$) are used in the definition of $E$. If we compute the Fourier coefficients using the FFT based on the "exact" ($\epsilon = 0$) *sampled* data, we find that the relative error in the estimates of the point of simple discontinuity and the associated jump at $x_1$ are of the order of $10^{-2}$ and $10^{-3}$, respectively. However, even when we set $\epsilon = 0.01$ and again use the FFT to compute the coefficients, we find the errors remain essentially unchanged from the case when $\epsilon = 0$.

**9. Reconstruction of $f$.** In a companion paper [6], we introduced and studied a class of $2\pi$-periodic, singular basis functions, which have special "built-in" discontinuities. In [6] it was proven that these functions can be used to construct a sequence of approximations to a discontinuous function, which converges exponentially to $f$ in the maximum norm. However, the construction procedure requires knowledge of the exact locations and magnitudes of all of the discontinuities in $f$ and its derivatives.

In this section we briefly summarize how the approximating sequence should be modified when only *estimates* of locations and magnitudes of the discontinuities in $f$ and its derivatives are known. In Appendix B, we outline how the main proof in [6] can be modified to show that the estimates we have obtained by the LSPE method are of sufficiently high quality so that we again obtain an approximating sequence which converges exponentially to $f$ in the maximum norm, for $x$ in the domain $\mathfrak{D}$. Here $\mathfrak{D}$ consists of the interval $[-\pi, \pi]$, with the union of certain "small" open intervals surrounding the points of discontinuity of $f$ removed. (The measure of $\mathfrak{D}$ converges exponentially to $2\pi$; see Appendix B for details.) In addition, the derivatives of this sequence converge exponentially to the corresponding derivatives of $f$, for $x \in \mathfrak{D}$.

The singular basis functions $\{S_n(x)\}$ are defined by

$$S_{2k}(x) \equiv \frac{2^{k-3/2}}{(2k)!} \sin(x)\,(1 - \cos(x))^{k-1/2} = \sum_{j=1}^{\infty} b_{2k,j} \sin(jx),,$$

(9.1)
$$S_{2k+1}(x) \equiv \frac{2^{k-1/2}}{(2k+1)!}\,(1 - \cos(x))^{k+1/2} = \frac{a_{2k+1,0}}{2} + \sum_{j=1}^{\infty} a_{2k+1,j} \cos(jx),$$

$$a_{2k+1,j} = (-1)^{k+1} \frac{4^{k+1}}{\pi} \frac{1}{\displaystyle\prod_{i=0}^{k} (4j^2 - (2i+1)^2)}, \quad b_{2k,j} = -j a_{2k+1,j}\,,$$

for $j = 0, 1, 2, \ldots$ , and $k = 0, 1, 2, \ldots$ . (For convenience in some of the formulas below, we also define $a_{2k,j} = b_{2k+1,j} = 0$, for $k \geq 0$.) It is straightforward to show that $S_m(x)$ is $C^{m-1}[-\pi, \pi]$, while the jump in its $m^{th}$ derivative at $x = 0$ is 1.

Now let $M$ be a nonnegative integer and let the $2\pi$-periodic function $f$ have possible discontinuities in $f^{(k)}$, for $0 \leq k \leq M$, at $x = x_s$, $s = 1, 2, \ldots, n$, where $-\pi < x_s \leq \pi$. We define

(9.2)
$$\tilde{S}_M^*(x) \equiv \sum_{k=0}^{M} \sum_{s=1}^{n} A_{k,s}^* S_k(x - x_s^*),$$

where the constants $\{A_{k,j}^*\}$ are determined recursively by

(9.3)
$$A_{k,s}^* = J_{k,s}^* - \sum_{i=0}^{k-1} A_{i,s}^* \left[ S_i^{(k)}(0) \right], \quad s = 1, 2, \ldots n, \quad k = 0, 1, \ldots, M.$$

Here $x_s^*$ and $J_{k,s}^*$ are the estimates of $x_s$ and $\left[ f^{(k)}(x_s) \right]$, respectively, determined by the LSPE method, as in sections 3, 5, and 6. (We note that, *if $x_s^* = x_s$ and if $J_{k,s}^* = \left[ f^{(k)}(x_s) \right]$, then $f(x) - \tilde{S}_M^*(x)$ will be $C^M[-\pi, \pi]$*, at least, and hence its Fourier series will converge at a faster rate than the Fourier series of $f$. See [6] for details.) Once $\tilde{S}_M^*(x)$ has been determined, we define the family of approximations $f_{M,N}^*$ to $f$ by

(9.4)
$$f_{M,N}^*(x) \equiv \tilde{S}_M^*(x) + \frac{a_0^{(M)}}{2} + \sum_{j=1}^{N} a_j^{(M)} \cos(jx) + b_j^{(M)} \sin(jx),$$

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$$a_j^{(M)} = a_j - \sum_{k=0}^{M} \sum_{s=1}^{n} A_{k,s}^* \left\{ a_{k,j} \cos(jx_s^*) - b_{k,j} \sin(jx_s^*) \right\},$$

(9.5)
$$b_j^{(M)} = b_j - \sum_{k=0}^{M} \sum_{s=1}^{n} A_{k,s}^* \left\{ a_{k,j} \sin(jx_s^*) + b_{k,j} \cos(jx_s^*) \right\},$$

$j = 0, 1, 2, ..., N$ .

To illustrate the reconstruction method described above, we reconsider Example 1. We reconstruct $f$ and a few of its derivatives using the first $2N+1$ of its Fourier coefficients. The estimates of the singularity locations and the associated jump parameters used are obtained by the LSPE method, with $M = 2$ and $N = 32$. Figure 6 illustrates the excellent agreement between $f$ (solid line) and $f_{2,32}^*$ (dashed line) . From Figs.7 and 8, it is evident that the first two derivatives of $f_{2,32}^*$ also agree, to within the plotting accuracy, with the corresponding derivatives of $f$. Figure 8 illustrates that there is a slight deterioration in the level of agreement between $f''$ (solid line) and $(f_{2,32}^*)''$ (dashed line) at points that are close to the points of singularity of $f''$. However, this deterioration is expected and can easily be eliminated by increasing $M$ and/or $N$.

**10. Conclusions, discussion, and future directions.** A simple, accurate, and robust method (the LSPE method) has been introduced and studied to estimate the locations and magnitudes of the jumps in a function $f$ and its derivatives, using only the information contained in the first $2N+1$ Fourier coefficients of $f$. These estimates can then be used with a simple class of periodic "singular basis functions" to construct a sequence of approximations which converges *exponentially* to $f$, and its derivatives, as $N \to \infty$, in the maximum norm, outside the union of a finite number of small open intervals that contain the points of singularity of $f$. The total measure of the union of all such "small" intervals approaches zero exponentially as $N \to \infty$. In particular, this implies that *the effects* of Gibbs phenomena can be *completely eliminated*, even when $f$ has several points of discontinuity. Also, the singularities of $f$ may be either points of simple discontinuity, or they may be points of higher order contact discontinuities. When compared with methods proposed by other investigators, the LSPE method was found to be at least as accurate and, often, significantly more accurate than other methods. Also, the LSPE method was found, in general, to be more robust and less sensitive to the effects of "closely spaced" singularities than other methods.

However, there are some issues connected with the LSPE method that we feel need further study. For example, a good rationale for the choice of the parameter $R$ in the definition of the objective function

(10.1)
$$E = \sum_{j=N+1-R}^{N} \omega_j E_j,$$

needs to be established. We have required that $N - R \gg 1$, in order for the asymptotic form of the Fourier coefficients to be valid, and that $2R$ is greater than the number of parameters being estimated. Intuitively, the freedom to choose "larger" values of $R$ has several advantages, including a smaller sensitivity of the $LSPE$ method to "small errors" in the Fourier coefficients. In most of the results reported in this paper, the choice of $R$ has been relatively ad-hoc, but some effort was made to keep it unchanged for each example considered. However, we observed that, in some cases (in Example 2, for instance), for different values of $N$ the convergence *rate* of the optimization routine seemed to be somewhat dependent on the choice of $R$. This sensitivity to the choice of $R$ has yet to be studied in any detail and all of our studies in this regard are preliminary in nature. It does seem reasonable, though, to conjecture that this sensitivity is due to the

decreasing magnitude of the Fourier coefficients with increasing $N$. For large $N$ and $M$, the limitation of having only a finite amount of precision in the coefficients causes "large" *relative* errors in the coefficients that are used. On the other hand, the idea of using larger values of $R$, for larger $N$ and $M$, in order to average out these relative errors, may not always be practical, as larger values of $R$ *may* cause a slowing in the convergence *rate* of the optimization method.

Also, a good criterion for the choice of the weights $\{w_j\}$ in the definition of $E$ needs to be determined. In particular, the proper assignment of the weights $\{w_j\}$ is crucial in the design of an *optimal* least-squares optimization method. All the results reported using the LSPE method (unless otherwise noted) were obtained using $w_j = j$. Some experimentation with assigning the weights shows that this choice is *not uniformly optimal*. However, all of our experimentation with $\{w_j\}$ has been preliminary, and more study is required to determine the *actual* sensitivity of the LSPE method to the choice of $w_j$.

Two important kinds of singularities in a function that are often encountered and which we have not addressed are *algebraic* and *logarithmic* singularities. Unlike Lipschitz functions, the Fourier coefficients of functions with these types of singularities *do not* have the same asymptotic form as for Lipschitz functions. Consequently, a new method to determine the locations and characteristics of the singularities of such a function need to be developed. Even after the singularities have been characterized, the basis functions $\{S_n(x)\}$ are no longer applicable, and some "new" basis functions with the appropriate algebraic or logarithmic singularity must be constructed. For an algebraic singularity, one possible candidate for a new basis function is

$$G(x,p) \equiv |\sin(x/2)|^p = \frac{a_0}{2} + \sum_{j=1}^{\infty} a_j \, \cos(jx),$$

where, for $p > -1$,

$$a_0 = \frac{2\,\Gamma((p+1)/2)}{\sqrt{\pi}\,\Gamma(1+p/2)}, \quad a_j = \frac{(-1)^j\,\Gamma(p+1)}{2^p\,\Gamma(1+j+p/2)\,\Gamma(1-j+p/2)}, \quad j \geq 1.$$

Here $\Gamma(z)$ is the usual Gamma function. Near $x = 0$, we have

$$G(x,p) = \frac{|x|^p}{2^p}\left\{1 + O\left(x^2\right)\right\},$$

and, hence, $G(x,p)$ could be used as a "basis function" to simulate a $p^{th}$ order *algebraic* singularity in a function $f$. For a function with a logarithmic singularity, the function

$$L(x) \equiv -\log|2\,\sin(x/2)| = \sum_{j=1}^{\infty} \frac{1}{j}\cos(jx),$$

might serve as an appropriate basis function, since, near $x = 0$,

$$L(x) = -\log|x| + O(x^2).$$

We also feel that many of the ideas we have presented for Fourier series can be extended to other orthogonal bases, as well. In particular, it is natural to expect "Gibbs-like" properties in "all" series using orthogonal sequences that approximate discontinuous functions. Gray and Pinsky [12] report a Gibbs like phenomenon for a Fourier-Bessel series of a piecewise smooth function, which displays a strange oscillation at the origin, quite unrelated to the local behavior of $f$ at that point. We feel that the problem of constructing a high order accurate sequence of approximations using information from a finite set of general orthogonal series coefficients can be addressed using extensions of several of the methods we have presented.

In addition, we feel that the ideas presented here will find useful applications in several different areas. Some particular applications currently being pursued include numerical shock capturing, image resolution enhancement, and time series analysis.

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**Appendix A. Convergence of initial estimates.** In this appendix we outline a proof of the rates of convergence as $N \to \infty$ of the estimates $\{\tilde{x}_s\}$ of the locations $\{x_s\}$ and the estimates $\{D_N(\tilde{x}_s)\}$ of the magnitudes $\{[f(x_s)]\}$ of the simple discontinuities of $f$, obtained from the extrema of the partial sums $\{D_N\}$, defined in Eq.(2.2).

Using Eq.(2.2) we can write

$$(A.1) \qquad \left( \frac{1}{\pi} \int_0^\pi \frac{\sin(u)}{u} du \right) D_N(x) = \sum_{j=1}^N \sin \left( \frac{j\pi}{N+1} \right) \{ b_j \cos(jx) - a_j \sin(jx) \}.$$

Then the condition that $dD_N/dx = 0$ implies

$$(A.2) \qquad 0 = \sum_{j=1}^N j \sin \left( \frac{j\pi}{N+1} \right) \{ a_j \cos(jx) + b_j \sin(jx) \}.$$

Using the asymptotic form (Eq.(3.1)) of the coefficients $\{a_j, b_j\}$, Eq.(A.2) can be written as

$$(A.3) \qquad \begin{aligned} 0 = \sum_{s=1}^n [f(x_s)] & \left\{ \sum_{j=1}^N \sin \left( \frac{j\pi}{N+1} \right) \sin(j(x - x_s)) \right\} - \\ & \sum_{s=1}^n [f'(x_s)] \left\{ \sum_{j=1}^N \frac{1}{j} \sin \left( \frac{j\pi}{N+1} \right) \cos(j(x - x_s)) \right\} + T_N(x), \end{aligned}$$

where

$$T_N(x) \equiv \sum_{j=1}^N \sin \left( \frac{j\pi}{N+1} \right) \{ \tilde{a}_j \cos(jx) + \tilde{b}_j \sin(jx) \},$$

with $\tilde{a}_j = O(j^{-2})$ and $\tilde{b}_j = O(j^{-2})$, as $j \to \infty$.

Let $\tilde{x}_k \equiv x_k + \epsilon_k$ denote the location of the extremum of $D_N$ nearest to $x_k$. We then write Eq.(A.3), evaluated at $x = \tilde{x}_k$, as

$$0 = [f(x_k)] \sum_{j=1}^N \sin \left( \frac{j\pi}{N+1} \right) \sin(j\epsilon_k)$$

$$+ \sum_{\substack{s=1 \\ s \neq k}}^n [f(x_s)] \left\{ \sum_{j=1}^N \sin \left( \frac{j\pi}{N+1} \right) \sin(j\Delta_{k,s}) \right\}$$

$$- [f'(x_k)] \sum_{j=1}^N \frac{1}{j} \sin \left( \frac{j\pi}{N+1} \right) \cos(j\epsilon_k)$$

$$(A.4) \qquad - \sum_{\substack{s=1 \\ s \neq k}}^n [f'(x_s)] \left\{ \sum_{j=1}^N \frac{1}{j} \sin \left( \frac{j\pi}{N+1} \right) \cos(j\Delta_{k,s}) \right\} + T_N(\tilde{x}_k),$$

where $\Delta_{k,s} \equiv x_k + \epsilon_k - x_s$, for $s \neq k$. Since $f$ is assumed to have only a finite number of points of discontinuity in the interval $(-\pi, \pi]$, we can assume that $|\Delta_{k,s}| \geq \tilde{\Delta} > 0$. Then, using elementary methods, we can show that, for any $\Delta \neq 0$,

$$(A.5) \qquad \sum_{j=1}^N \frac{1}{j^m} \sin \left( \frac{j\pi}{N+1} \right) \sin(j\Delta) = O(N^{-1}), \quad m \geq 0,$$

$$\text{(A.6)} \qquad \sum_{j=1}^{N} \frac{1}{j^m} \sin\left(\frac{j\pi}{N+1}\right) \cos\left(j\Delta\right) = O(N^{-1}), \quad m \geq 1,$$

as $N \to \infty$. Using these results, we see that the second and fourth terms on the right side of Eq.(A.4) are each $O(N^{-1})$, as $N \to \infty$. Also, $T_N(\tilde{x}_k) = O(N^{-1})$, as $N \to \infty$, since the coefficients $\{\tilde{a}_j\}$ and $\{\tilde{b}_j\}$ are each $O(j^{-2})$, as $j \to \infty$. If we now assume that $j\epsilon_k = o(1)$, as $N \to \infty$, for all $j \leq N$, we can write Eq.(A.4) as

$$0 = \epsilon_k \cdot \left(1 + O\left((N\epsilon_k)^2\right)\right) \cdot [f(x_k)] \sum_{j=1}^{N} j \sin\left(\frac{j\pi}{N+1}\right) -$$

$$\text{(A.7)} \qquad [f'(x_k)] \cdot \left(1 + O\left((N\epsilon_k)^2\right)\right) \cdot \sum_{j=1}^{N} \frac{1}{j} \sin\left(\frac{j\pi}{N+1}\right) + O(N^{-1}).$$

We now use the facts that

$$\sum_{j=1}^{N} j \sin\left(\frac{j\pi}{N+1}\right) = \frac{(N+1)^2}{\pi} + O\left(1\right),$$

$$\text{(A.8)} \qquad \sum_{j=1}^{N} \frac{1}{j} \sin\left(\frac{j\pi}{N+1}\right) = \int_0^{\pi} \frac{\sin(x)}{x} dx + O\left(\frac{1}{N}\right),$$

as $N \to \infty$, to write Eq.(A.7) as

$$\text{(A.9)} \qquad \epsilon_k = \frac{\pi}{(N+1)^2} \int_0^{\pi} \frac{\sin(x)}{x} dx \cdot \frac{[f'(x_k)]}{[f(x_k)]} + O(N^{-3}),$$

as $N \to \infty$. From Eq.(A.9) and the definition of $\epsilon_k$, we see that $\tilde{x}_k = x_k + O(N^{-2})$, as $N \to \infty$, as asserted in Theorem 2.1.

Also, using some of the same steps that led to Eq.(A.4), we can write

$$\text{(A.10)} \qquad \text{Si}(\pi) \cdot D_N(\tilde{x}_k) = [f(x_k)] \left\{ \sum_{j=1}^{N} j^{-1} \sin\left(\frac{j\pi}{N+1}\right) \right\} \left(1 + O\left((N\epsilon_k)^2\right)\right)$$

$$+ \sum_{\substack{s=1 \\ s \neq k}}^{n} [f(x_s)] \left\{ \sum_{j=1}^{N} j^{-1} \sin\left(\frac{j\pi}{N+1}\right) \cos(j\Delta_{k,s}) \right\}$$

$$+ \sum_{s=1}^{n} [f'(x_s)] \left\{ \sum_{j=1}^{N} \frac{1}{j^2} \sin\left(\frac{j\pi}{N+1}\right) \sin(j\Delta_{k,s}) \right\} - \dots .$$

Using Eqs.(A.5) and (A.6), we find that each of the terms beyond the first on the right side of Eq.(A.10) is $O(N^{-1})$, as $N \to \infty$. Then, using Eq.(A.8), we find that Eq.(A.10) can be written as

$$D_N(\tilde{x}_k) = [f(x_k)] + O(N^{-1}),$$

as stated in Theorem 2.1.

**Appendix B. Exponential convergence.** We now outline a proof that the sequence $\left\{ f^*_{M,\lambda M} \right\}$ converges exponentially to $f$ in the maximum norm, outside the union of a finite number of small open intervals that contain the points of singularity of $f$.

To establish this exponential convergence, we first define the error terms

$$E_{M,N}(x) \equiv f(x) - f^*_{M,N}(x) = E^{(1)}_{M,N}(x) + E^{(2)}_{M,N}(x),$$

where

(B.1) $$E^{(1)}_{M,N}(x) \equiv f(x) - f_{M,N}(x), \quad E^{(2)}_{M,N}(x) \equiv f_{M,N}(x) - f^*_{M,N}(x).$$

Here $f_{M,N}$ is defined by the right side of Eq.(9.4) with $x^*_s$ and $J^*_{k,s}$ replaced by $x_s$ and $\left[ f^{(k)}(x_s) \right]$, respectively, in the definitions (9.2)-(9.5). From the results of [6], $E^{(1)}_{M,\lambda M}(x)$ decays to zero exponentially, as $M \to \infty$. To show that $E^{(2)}_{M,\lambda M}(x)$ also decays to zero exponentially, we note first that, from its definition,

(B.2) $$f^*_{M,N}(x) \equiv \frac{a_0}{2} + \sum_{j=1}^{N} a_j \cos(jx) + b_j \sin(jx) + \sum_{k=0}^{M} \sum_{s=1}^{n} A^*_{k,s} \, Y_{k,N}(x - x^*_s),$$

where

(B.3) $$Y_{k,N}(x) \equiv \sum_{j=N+1}^{\infty} a_{k,j} \cos(jx) + b_{k,j} \sin(jx).$$

Thus, it follows from Eqs.(B.1), (B.2), and (9.2)-(9.5) that

$$E^{(2)}_{M,N}(x) = \sum_{k=0}^{M} \sum_{s=1}^{n} \left( A_{k,s} \, Y_{k,N}(x - x_s) - A^*_{k,s} \, Y_{k,N}(x - x^*_s) \right).$$

Here the constants $\{A_{k,s}\}$ are defined by Eq.(9.3) with $J^*_{k,s}$ replaced by $\left[ f^{(k)}(x_s) \right]$. To facilitate our proof below, we rewrite $E^{(2)}_{M,N}(x)$ as

(B.4) $$E^{(2)}_{M,N}(x) = E^{(2,1)}_{M,N}(x) + E^{(2,2)}_{M,N},$$

where

(B.5) $$E^{(2,1)}_{M,N}(x) = \sum_{k=0}^{M} \sum_{s=1}^{n} A_{k,s} \left\{ Y_{k,N}(x - x_s) - Y_{k,N}(x - x^*_s) \right\},$$

and

(B.6) $$E^{(2,2)}_{M,N}(x) = \sum_{k=0}^{M} \sum_{s=1}^{n} \left\{ A_{k,s} - A^*_{k,s} \right\} Y_{k,N}(x - x^*_s).$$

In order to show that $E^{(2)}_{M,\lambda M}(x)$ decays to zero exponentially, as $M \to \infty$, it suffices to show that both $E^{(2,1)}_{M,\lambda M}(x)$ and $E^{(2,2)}_{M,\lambda M}(x)$ decay to zero exponentially, as $M \to \infty$.

Using Eqs.(6.3)-(6.4), we can write

(B.7) $$x^*_s - x_s = \frac{\psi_{M,s}}{N^{M+2}} \left( 1 + O\left( 1/N \right) \right),$$

(B.8) $$J^*_{k,s} - \left[ f^{(k)}(x_s) \right] = \frac{\alpha_{M,k,s}}{N^{M+1-k}} \left( 1 + O\left( 1/N \right) \right), \text{ as } N \to \infty,$$

for $s = 1, 2, ..., n$, and $k = 0, 1, .., M$. Here $\psi_{M,s}$ and $\alpha_{M,k,s}$ are certain constants.

We first outline a proof that $E_{M,N}^{(2,1)}$ decays exponentially to zero. From Eqs.(9.1), it follows that

$$(B.9) \qquad |a_{k,j}| \leq \frac{c_1}{j^{k+1}}, \text{ and } |b_{k,j}| \leq \frac{c_2}{j^{k+1}},$$

where $c_1$ and $c_2$ are constants independent of $k$ and $j$. Therefore, it follows from Eq.(B.3) that there exists a constant $C_1$, independent of $k$ and $N$, such that

$$(B.10) \qquad \max_{-\pi \leq x \leq \pi} |Y_{k,N}| \leq C_1 \sum_{j=N+1}^{\infty} \frac{1}{j^{k+1}} \leq \frac{C_1}{k} \frac{1}{N^k}, \text{ for } k \geq 1,$$

which follows easily by the integral comparison test. Using Eq.(B.3), Eq.(B.7), the integral comparison test, and Taylor's theorem, we obtain

$$(B.11) \qquad |Y_{k,N}(x - x_s^*) - Y_{k,N}(x - x_s)| \leq C_2 \frac{|\overline{\psi}_{M,s}|}{N^{M+2}} \frac{1}{k-1} \frac{1}{N^{k-1}},$$

for $s = 1, 2, ..., n$, $k = 2, .., M$, and for

$$(B.12) \qquad |x - x_s^*| \geq O(\psi_{M,s} N^{-M-2}).$$

Here, $\overline{\psi}_{M,s} = \psi_{M,s} (1 + O(1/N))$, and $C_2$ is a constant independent of $M$ and $k$. We now assume that there exist some positive constants $\delta_1, \delta_2, \delta_3, \Delta_1, \Delta_2$, and $\Delta_3$, such that the following bounds hold:

$$|\overline{\alpha}_{M,k,s}| \leq \Delta_1 M \delta_1^k k!,$$

$$|A_{k,s}| \leq \Delta_2 \delta_2^k k!, \text{ and}$$

$$(B.13) \qquad |\overline{\psi}_{M,s}| \leq \Delta_3 \delta_3^M M!, \text{ for } s = 1, ..., n.$$

The restrictions (B.13) are mild, and are motivated by a similar study in [6]. Then, using Eqs.(B.11) and (B.13), we find that, for $k \geq 2$,

$$|A_{k,s}| \cdot |Y_{k,N}(x - x_s) - Y_{k,N}(x - x_s^*)| \leq \tilde{d}_1 \delta_2^k N \frac{\delta_3^M M!}{N^{M+2}(k-1)},$$

where $\tilde{d}_1$ is a constant. Using Stirling's approximation for $M!$ and setting $N = \lambda M$, we find

$$(B.14) \qquad \sum_{k=0}^{M} \sum_{s=1}^{n} |A_{k,s}| \cdot |Y_{k,N}(x - x_s) - Y_{k,N}(x - x_s^*)| \leq d_2 \sqrt{M} \left( \frac{\delta_2 \delta_3}{\lambda e} \right)^M,$$

where $d_2$ is a constant independent of $M$. Thus, for any fixed values of $\delta_2$ and $\delta_3$ (with $\delta_2 \delta_3 > e$), we can select $\lambda$ large enough so that $(\delta_2 \delta_3)/(\lambda e) < 1$. Consequently, $E_{M,\lambda M}^{(2,1)}(x)$ decays to zero exponentially, as $M \to \infty$.

We now consider $E_{M,\lambda M}^{(2,2)}(x)$. From the definitions of $A_{k,s}^*$ and $A_{k,s}$, and Eqs.(B.8), it follows that

$$(B.15) \qquad |A_{k,s}^* - A_{k,s}| \leq \frac{|\overline{\alpha}_{M,k,s}|}{N^{M+1-k}} + \sum_{\substack{i=2 \\ i \text{ even}}}^{k} \frac{|\overline{\alpha}_{M,k-i,s}|}{N^{M+1+i-k}} \cdot |\beta_{k,k-i}|,$$

where $\alpha_{M,-1,s} = 0$, $\beta_{k,k-2} = [S_{k-2}^{(k)}(0)]$, and, in general, $\beta_{k,k-i}$ is a function of the jumps $[S_j^{(k)}(0)]$, $j = 1, ..., k$. We now conjecture that the following bound holds for $\beta_{k,k-i}$ :

$$(B.16) \qquad |\beta_{k,k-i}| \leq \frac{k!}{(k-i)!} \left(\frac{k}{e}\right)^i.$$

Although we do not have an analytical proof for this bound, it has been verified using Mathematica [22] for $0 \leq i \leq k \leq 300$. Therefore, using Eqs.(B.13) and (B.16), and assuming $N > M/(e\delta_1)$, it follows from Eq.(B.15) that

$$(B.17) \qquad |A_{k,s}^* - A_{k,s}| \leq C_3 \frac{M\delta_1^k k!}{N^{M+1-k}},$$

where $C_3$ is a constant independent of $M$ and $k$. Using Eqs.(B.17), (B.10), and (B.13) we obtain

$$|A_{k,s} - A_{k,s}^*| \cdot |Y_{k,N}(x - x_s^*)| \leq \tilde{d}_2 \frac{M \, \delta_1^k \, (k-1)!}{N^{M+1}}.$$

Therefore, using Stirling's approximation for $M!$ and setting $N = \lambda M$, we find

$$(B.18) \qquad \sum_{k=0}^{M} \sum_{s=1}^{n} |A_{k,s} - A_{k,s}^*| \cdot |Y_{k,N}(x - x_s^*)| \leq d_1 M^{3/2} \left(\frac{\delta_1}{\lambda \, e}\right)^M.$$

As a consequence, for a fixed $\delta_1$, if we select $\lambda$ such that $\lambda > \delta_1/e$, $E_{M,\lambda M}^{(2,2)}(x)$ decays to zero exponentially, as $M \to \infty$.

It now follows from Eqs.(B.4)-(B.6), (B.14) and (B.18) that

$$(B.19) \qquad \left|E_{M,\lambda M}^{(2)}(x)\right| \leq d_1 M^{3/2} \left(\frac{\delta_1}{\lambda \, e}\right)^M + d_2 \sqrt{M} \left(\frac{\delta_2 \delta_3}{\lambda \, e}\right)^M,$$

where $d_1$, $d_2$ are certain constants. From equation (B.19) we see that, for any fixed values of $\delta_1, \delta_2$ and $\delta_3$, if we select $\lambda$ so that

$$(B.20) \qquad \lambda > \max(\delta_1/e, \ \delta_2\delta_3/e),$$

then $E_{M,\lambda M}^{(2)}(x)$ decays to zero exponentially, as $M \to \infty$.

Consequently, $E_{M,\lambda M}(x)$ decays to zero exponentially in the maximum norm for $x$ in the domain $\mathfrak{D}$. Here $\mathfrak{D}$ consists of the interval $[-\pi, \pi]$, with the union of a finite number of "small" open intervals, $I_s$, for $s = 1, 2, ..., n$, surrounding the points of singularity of $f$, removed. In order to show that the total measure of the union of these "small" open intervals, $I_s$, decays to zero exponentially, we observe from Eq.(B.12) that the length $L_s$ of the interval $I_s$ satisfies

$$L_s \leq O(\overline{\psi}_{M,s} \, N^{-M-2}).$$

Using the bound on $\overline{\psi}_{M,s}$ from Eqs.(B.13) we find that, for $N = \lambda M$ and for large $M$,

$$L_s \leq O\left(M^{-3/2} \left(\frac{\delta_3}{\lambda e}\right)^M\right).$$

Thus, it follows that the total measure, $\sum_{s=1}^{n} L_s$, of the union of the intervals goes to zero exponentially, as $M \to \infty$.

Finally, we show that $\left(f^*_{M,\lambda M}(x)\right)'$ converges exponentially to $f'(x)$ in the maximum norm in the domain $\mathfrak{D}$, as $M \to \infty$. We observe that, from the results of [6] and from Eqs.(B.1), (B.4), (B.5) and (B.6), it suffices to show that both $\left(E^{(2,1)}_{M,\lambda M}(x)\right)'$ and $\left(E^{(2,2)}_{M,\lambda M}(x)\right)'$ decay to zero exponentially, as $M \to \infty$. Using Eqs.(B.3), (B.13), the integral comparison test, and Taylor's theorem it follows that

(B.21)
$$\left|Y'_{k,N}(x - x^*_s) - Y'_{k,N}(x - x_s)\right| \leq C_4 \frac{|\overline{\psi}_{M,s}|}{N^{M+2}} \frac{1}{k-2} \frac{1}{N^{k-2}},$$

and

(B.22)
$$\max_{x \in \mathfrak{D}} \left|Y'_{k,N}(x)\right| \leq C_5 \frac{1}{k-1} \frac{1}{N^{k-1}},$$

for $k = 3, ..., M$. Here, $C_4$ and $C_5$ are constants independent of $k$ and $M$. Therefore, using Stirling's approximation for $M!$ and setting $N = \lambda M$, it follows that

(B.23)
$$\left|\left(E^{(2,1)}_{M,\lambda M}(x)\right)'\right| \leq M^{3/2} \left(\frac{\delta_2 \delta_3}{\lambda e}\right)^M,$$

and

(B.24)
$$\left|\left(E^{(2,2)}_{M,\lambda M}(x)\right)'\right| \leq M^{5/2} \left(\frac{\delta_1}{\lambda e}\right)^M.$$

Thus, assuming that $\lambda$ satisfies the condition (B.20), it follows that $\left(f^*_{M,\lambda M}(x)\right)'$ converges to $f'(x)$ exponentially in the maximum norm in the domain $\mathfrak{D}$, as $M \to \infty$. Using mathematical induction, it follows that the first $l$ derivatives of $f^*_{M,\lambda M}(x)$ converge exponentially to the corresponding derivatives of $f(x)$, as $M \to \infty$. This completes our proof.
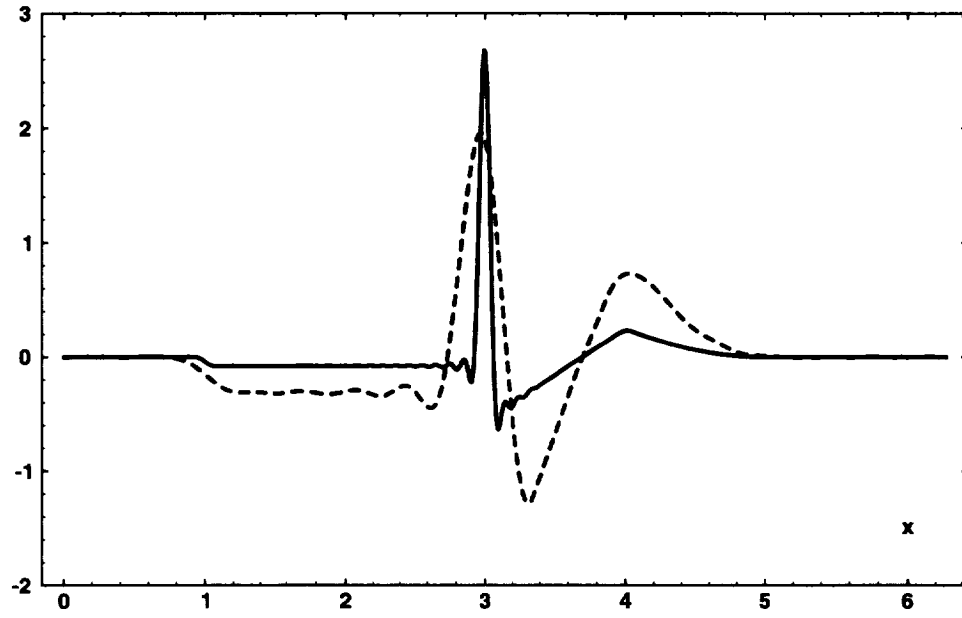
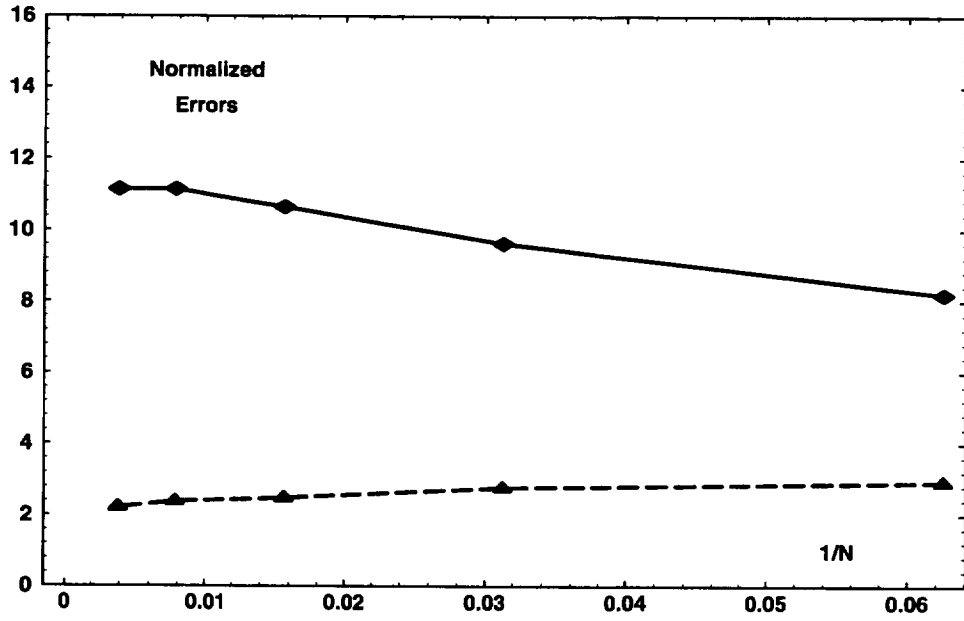FiG. 1. *Plots of $D_N(x)$ for Example 1 using $N = 16$ (dashed line) and $N = 64$ (solid line).*

FIG. 2. *The normalized errors* $N^2 |\tilde{x}_1 - x_1|$ *(solid line), obtained from* $D_N(x)$*, and* $N^2 |x_1^* - x_1|$ *(dashed line), obtained from the LSPE method, for Example* 1, *plotted as functions of* $1/N$.
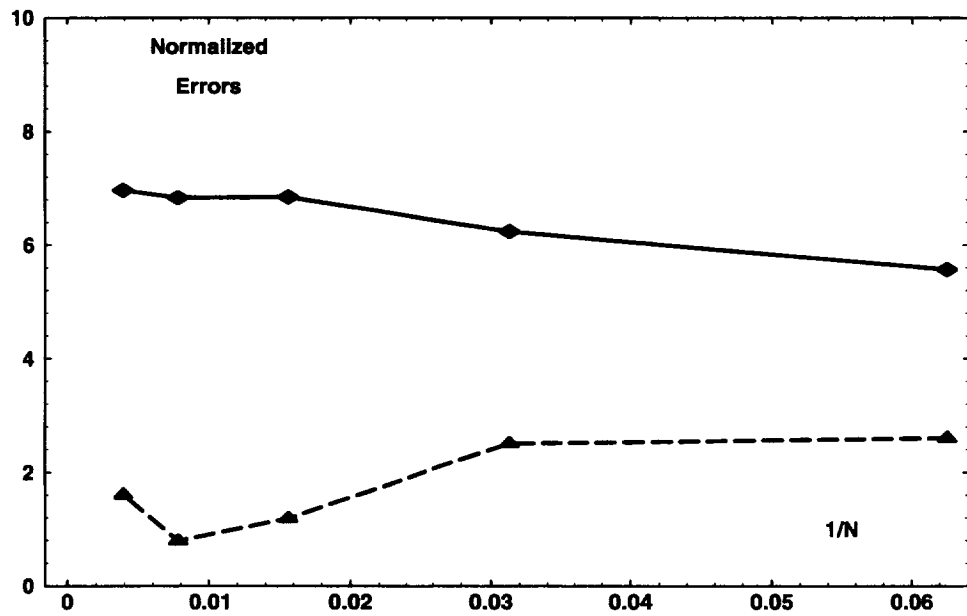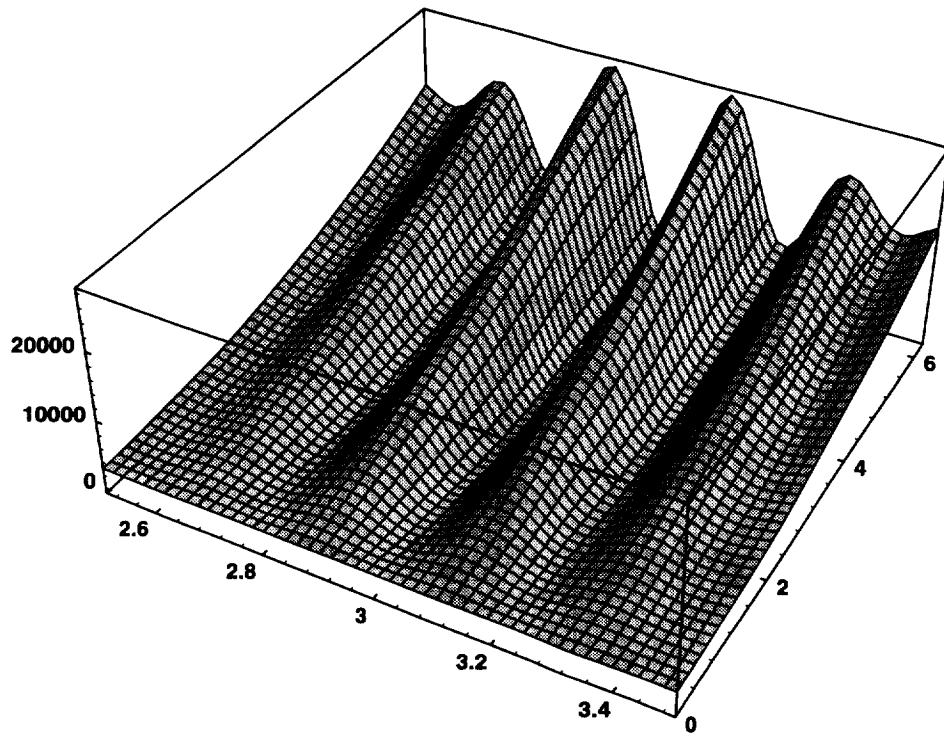
FIG. 3. *The normalized errors* $N |D_N(\bar{x}_1) - [f(x_1)]|$ *(solid line), obtained from* $D_N(x)$, *and* $N^2 \left| J^*_{0,1} - [f(x_1)] \right|$ *(dashed line), obtained from the LSPE method, for Example 1, plotted as functions of* $1/N$.

FIG. 4. *A surface plot of the error function* $E$ *(see Eq.(3.3)) for Example 1, as a function of* $\hat{x}_1$ *and* $\hat{J}_{0,1}$, *near the minimum of* $E$. *Here* $N = 32$, $R = 12$, *and* $\omega_j = j$.
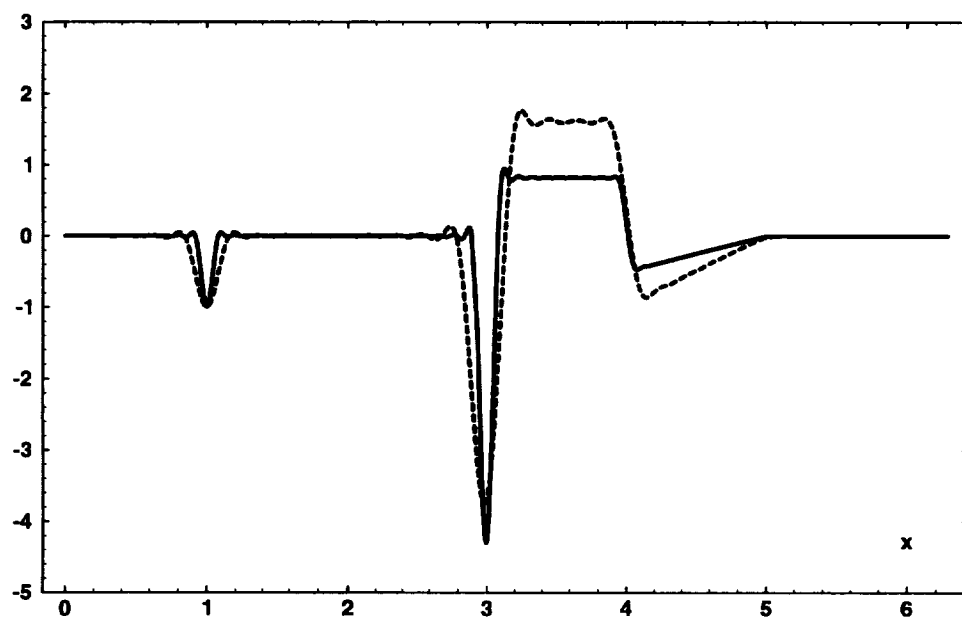
FIG. 5. *Plots of $D_{1,N}(x)$ for Example 1 using $N = 32$ (dashed line) and $N = 64$ (solid line).*
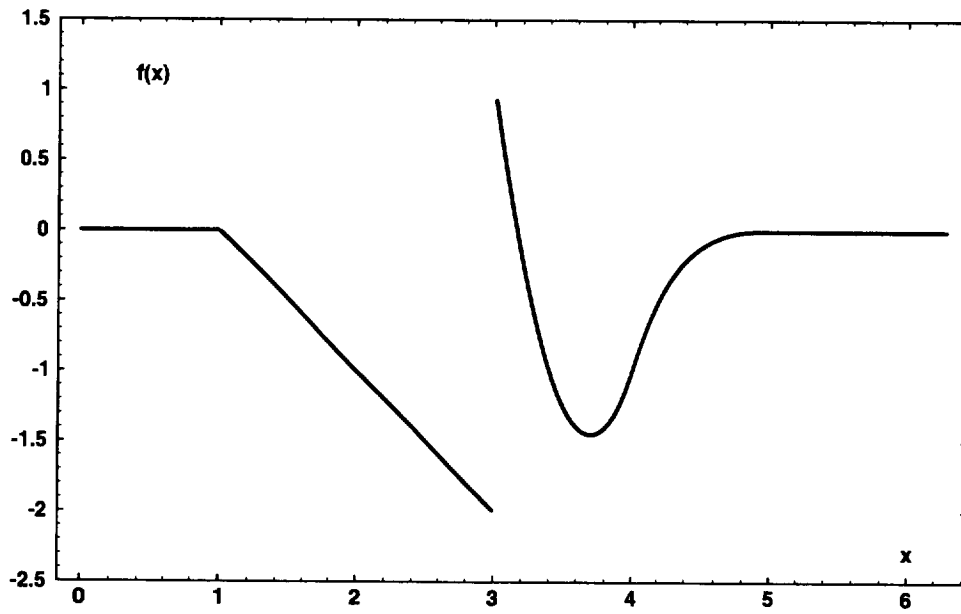
FIG. 6. *The reconstructed approximation* $f_{2,32}^*(x)$ *(dashed line) for the function* $f(x)$ *(solid line) of Example 1, using the parameter estimates obtained by the LSPE method with* $M = 2$ *and* $N = 32$.
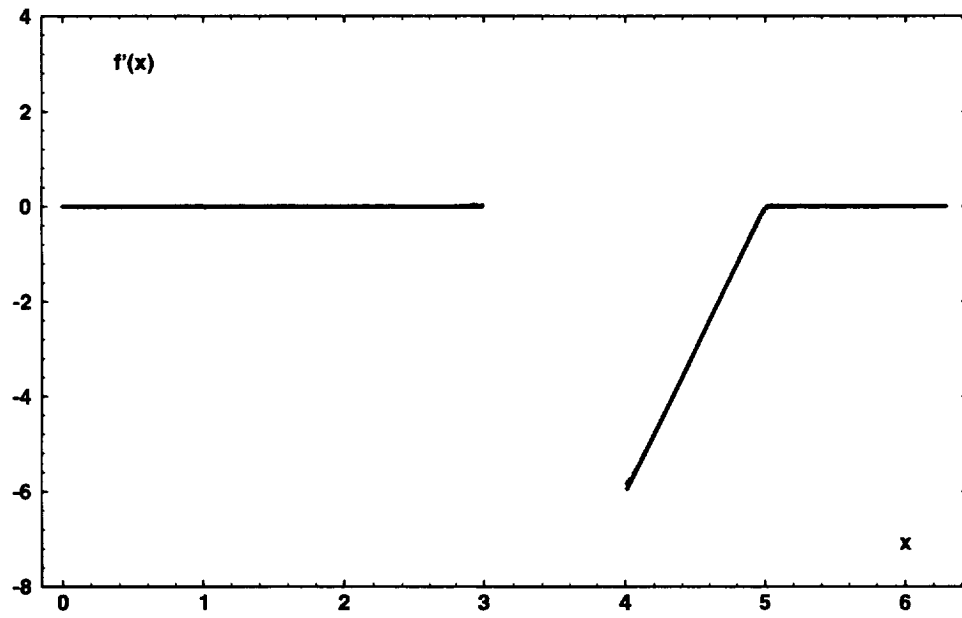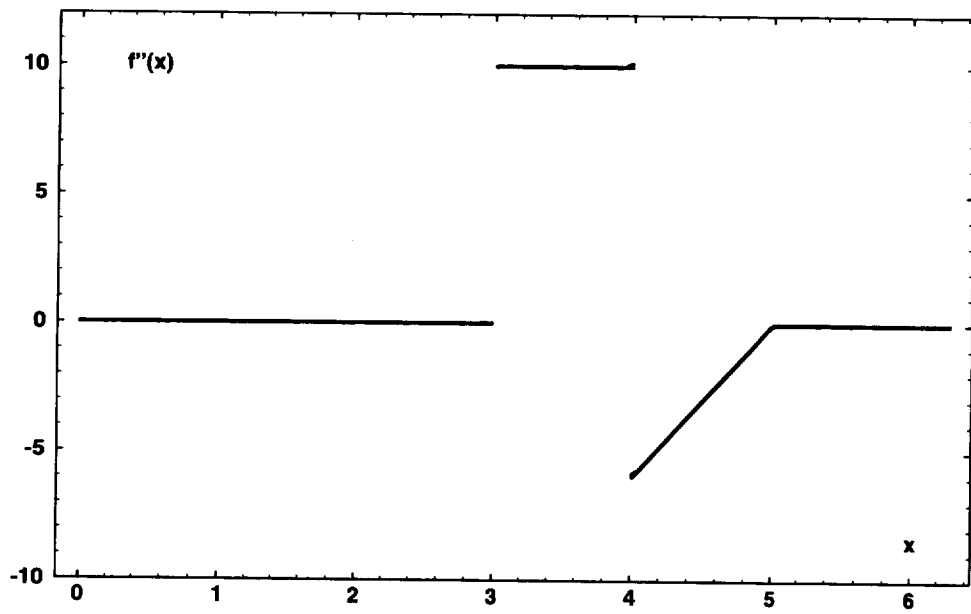
FIG. 7. *The reconstructed approximation* $\left(f_{2,32}^*(x)\right)'$ *(dashed line) for the function* $f'(x)$ *(solid line) of Example 1, using the parameter estimates obtained by the LSPE method with* $M = 2$ *and* $N = 32$.

FIG. 8. *The reconstructed approximation* $\left(f_{2,32}^*(x)\right)''$ *(dashed line) for the function* $f''(x)$ *(solid line) of Example 1, using the parameter estimates obtained by the LSPE method with* $M = 2$ *and* $N = 32$.

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**13. ABSTRACT** *(Maximum 200 words)*

The problem of accurately reconstructing a piece-wise smooth, $2\pi$-periodic function $f$ and its first few derivatives, given only a truncated Fourier series representation of $f$, is studied and solved. The reconstruction process is divided into two steps. In the first step, the first $2N + 1$ Fourier coefficients of $f$ are used to approximate the locations and magnitudes of the discontinuities in $f$ and its first $M$ derivatives. This is accomplished by first finding initial estimates of these quantities based on certain properties of Gibbs phenomenon, and then refining these estimates by fitting the asymptotic form of the Fourier coefficients to the given coefficients using a least-squares approach. It is conjectured that the locations of the singularities are approximated to within $O\left(N^{-M-2}\right)$, and the associated jump of the $k^{th}$ derivative of $f$ is approximated to within $O\left(N^{-M-1+k}\right)$, as $N \to \infty$, and the method is robust. These estimates are then used with a class of singular basis functions, which have certain "built-in" singularities, to construct a new sequence of approximations to $f$. Each of these new approximations is the sum of a piecewise smooth function and a new Fourier series partial sum. When $N$ is proportional to $M$, it is shown that these new approximations, and their derivatives, converge exponentially in the maximum norm to $f$, and its corresponding derivatives, except in the union of a finite number of small open intervals containing the points of singularity of $f$. The total measure of these intervals decreases exponentially to zero as $M \to \infty$. The technique is illustrated with several examples.

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