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Acceleration of algebraically-converging Fourier series when the coefficients have series in powers of $1/n$

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ABSTRACT

If the coefficients in a Fourier cosine series, $f(x) \approx f_N = \sum_{n=0}^{\infty} a_n \cos(nx)$, decrease as a small negative power of n, then one may need millions of terms to sum the series to high accuracy. We show that if the a_n are known analytically and have a power series in $1/n$, then it is straightforward to approximate $f(x)$ as a series of what we shall the Lanczos–Krylov (LK) functions. (We describe the similar methodology for sine series; general Fourier series are merely the sum of a cosine series with a sine series and thus are implicitly handled, too.) For cosine coefficients that involve only even powers of n and sine coefficients that are functions of odd powers of n, the LK functions may be expressed in terms of Bernoulli polynomials. The LK functions for cosine coefficients involving odd powers of n and for sine coefficients in even powers of n are not known explicitly; these are also known as "Clausen functions". We provide rapidly convergent series to compute these Clausen functions to high accuracy. Our method includes the "endpoint subtraction" ideas of Lanczos and Krylov, but is more general. The sum $\sum_{n=1}^{\infty} (\pm 1)^{n+1} (1/(n+\lambda)) \cos(nx)$, where $\lambda > 0$ is a constant, arises in phase transitions in absorbed monolayers on metal surfaces. It is easily summed by our method, which correctly incorporates the logarithmic singularities at $x = \pm\pi$.

1. Introduction

1.1. The basic idea

Slowly-convergent Fourier series are a widespread bain in science and engineering [25]. A nasty exemplar is

$$\chi(x;\lambda) \equiv \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n+\lambda} \cos(nx) \tag{1}$$

which arises in the phase transitions of absorbed submonolayers on metal surfaces [40], and is also the real part of a special case of the "Lerch zeta-function" in mathematics. If the series is truncated after the N-th term, the error falls only as fast as $1/N$ over the entire interval except in zones of width $O(1/N)$ near $x = \pm\pi$ where the error is always $O(1)$, the Gibbs Phenomenon.

Much effort has been devoted to defeating the Gibbs Phenomenon as again reviewed most recently in [25]. Individual articles on accelerating Fourier series include [20,19,18,17,41,9,5,49,7,14,10–12,24,23,4,1,3,2,21,28,27,26,22,43–46,16,29,30,36–39,42,47,48,50,51]. It is obviously impossible to summarize such a great body of work without writing a lengthy review article. Install, we shall relate our method to existing work as we proceed.

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Our key assumption is that the Fourier coefficients a_n of the Fourier series for $f(x)$ have a power series in inverse powers of n as $n \to \infty$:

$$a_n \sim (-1)^{n+1} \sum_{k=1}^{\infty} \xi_k n^{-k}, \quad n \to \infty \tag{2}$$

(The alternating sign is convenient in this implicit definition of the ξ_k because we assume that the slow convergence is caused by singularities at $x = \pm\pi$, in which case the Fourier coefficients alternate in sign, at least asymptotically.) It is not necessary that the series be convergent (although it is for $\chi(x;\lambda)$); an asymptotic-but-divergent series will do just as well. Specializing to a cosine series for the moment, choose M to be a large but otherwise arbitrary positive integer and write

$$f(x) = s_M + r_M(x) \tag{3}$$

where s_M is the usual partial sum

$$s_M = \sum_{n=1}^{M} a_n \cos(nx) \tag{4}$$

and the "tail" is

$$r_M(x,\lambda) = \sum_{n=M+1}^{\infty} a_n \cos(nx) \tag{5}$$

Inserting the asymptotic approximation only in the "tail" $r_M(x)$ gives

$$\begin{aligned} f(x) &= s_M + \sum_{n=M+1}^{\infty} \left\{ (-1)^{n+1} \sum_{k=1}^{\infty} \xi_k n^{-k} \right\} \cos(nx) = s_M + \sum_{k=1}^{\infty} \xi_k \left\{ \sum_{n=M+1}^{\infty} (-1)^{n+1} \frac{1}{n^k} \cos(nx) \right\} \\ &= s_M + \sum_{k=1}^{\infty} \xi_k \{ \mathcal{C}_k(x) - \mathcal{C}_{k,M}(x) \} = \left\{ s_M - \sum_{k=1}^{\infty} \xi_k \mathcal{C}_{k,M}(x) \right\} + \sum_{k=1}^{\infty} \xi_k \mathcal{C}_k(x) \\ &= \sum_{n=1}^{M} \left\{ a_n - (-1)^{n+1} \sum_{k=1}^{\infty} \frac{\xi_k}{n^k} \right\} \cos(nx) + \sum_{k=1}^{\infty} \xi_k \mathcal{C}_k(x) \end{aligned} \tag{6}$$

where we have defined

$$\mathcal{C}_k(x) = \sum_{n=1}^{\infty} (-1)^{n+1} n^{-k} \cos(nx) \tag{7}$$

and $\mathcal{C}_{k,M}(x)$ is the partial sum of these series,

$$\mathcal{C}_{k,M}(x) = \sum_{n=1}^{M} (-1)^{n+1} n^{-k} \cos(nx) \tag{8}$$

The crucial point is that these "Lanczos–Krylov" (LK) functions can be evaluated in closed form either as Bernoulli polynomials (for even k) or by the method derived in the appendix. It is only necessary for the asymptotic approximation to the Fourier coefficients to be accurate for $n > M$ where M can be chosen as large as necessary.

The method is similar for sine series except that we must use the "sine" LK functions $\mathcal{S}_k(x)$ defined below.

In practice, the series in k must be truncated. If the sum in (6) includes the $k = K$ term, then the leading Fourier coefficient of the first neglected term is

$$\xi_{K+1} \frac{1}{(M+1)^{K+1}} \tag{9}$$

Obviously, the error can be made arbitrarily small by choosing sufficiently large M and K. To avoid the bother of computing a large number of the LK functions $\mathcal{C}_k(x)$, we recommend choosing $M \gg K$, that is, using a truncation in s_M and $\mathcal{C}_{k,M}$ which is much larger than the truncation K in the order of the LK functions. (In the example below, for example, we chose $K = 4$ and $M = 50$.)

If the series for a_n in powers of $1/n$ is convergent, then (6) is *exact*. If the series is only asymptotic, then the approximation for $f(x;\lambda)$ is asymptotic, too. However, because M is arbitrary where M is the cutoff between explicit summation and the use of the asymptotic expansion for a_n, the error for $f(x)$ can be made as small as we wish by choosing sufficiently large M.

There is no loss of generality in discussing cosine and sine series separately because an arbitrary function $f(x)$ can always be split into its parts which are symmetric and antisymmetric about the origin via

$$S(x) \equiv \frac{1}{2}(f(x) + f(-x)), \quad A(x) \equiv \frac{1}{2}(f(x) - f(-x)) \tag{10}$$

where even parity means $S(-x) = S(x)$ for all x and $A(x)$ is antisymmetric in the sense that $A(-x) = -A(x)$ for all x. Then $S(x)$ and $A(x)$ can be approximated by cosine and sine series respectively:

$$S(x) = a_0 + \sum_{n=1}^{\infty} a_n \cos(nx), \quad A(x) = \sum_{n=1}^{\infty} b_n \sin(nx) \tag{11}$$

where

$$f(x) = S(x) + A(x) \tag{12}$$

2. Non-periodic $f(x)$ and Bernoulli polynomials

In many applications, the Fourier series converges slowly only because $f(x)$ is not a periodic function. The Fourier series, which is composed entirely of functions that are individually periodic with period 2π, is forced to converge to the *piecewise* smooth *periodic* function $\hat{f}(x)$ defined by

$$\hat{f}(x) \equiv \begin{cases} f(x), & x \in [-\pi, \pi] \\ f(\mathrm{mod}(x+\pi, 2\pi) - \pi), & |x| > \pi \end{cases} \tag{13}$$

which is to say that $\hat{f}(x)$ is extended to $|x| > \pi$ by the periodicity condition $\hat{f}(x + 2\pi) = \hat{f}(x)$ for all x. The periodized function $\hat{f}(x)$ has discontinuities in the function itself or its derivatives at $x \pm \pi$ which force its Fourier series to decay very slowly with n.

Lanczos and Krylov [6,31,32] independently observed in the mid-twentieth century that the Fourier coefficients of such "piecewise analytic" functions have a "Fourier coefficient asymptotic expansion" (FACE) [34,35,13] in inverse powers of n.

$$a_n \sim \frac{1}{\pi} \sum_{j=0}^{J} (-1)^{n+j} \left(\frac{f^{(2j+1)}(\pi) - f^{(2j+1)}(-\pi)}{n^{2j+2}} \right) + O(n^{-(2J+4)}), n \to \infty, \text{ fixed } J \tag{14}$$

$$b_n \sim \frac{1}{\pi} \sum_{j=0}^{J} (-1)^{n+1+j} \left(\frac{f^{(2j)}(\pi) - f^{(2j)}(-\pi)}{n^{2j+1}} \right) + O(n^{-(2J+3)}), n \to \infty, \text{ fixed } J \tag{15}$$

Note that only *even* powers appear in the series for the cosine coefficients and only *odd* powers of n in the expansion of the sine coefficients.

It was known to Lanczos and Krylov that these LK functions are piecewise shifted Bernoulli polynomials. The first few cases are given explicitly in Table 1. The general form is

$$\mathcal{S}_{2K-1}(x) \equiv \sum_{n=1}^{\infty} (-1)^{n+1} n^{-(2K-1)} \sin(nx) \tag{16}$$

$$= (-1)^K \frac{2^{2K-2} \pi^{2K-1}}{(2K-1)!} B_{2K-1}\left(\frac{x+\pi}{2\pi}\right) \tag{17}$$

$$\mathcal{C}_{2K}(x) \equiv \sum_{n=1}^{\infty} (-1)^{n+1} n^{-2K} \cos(nx) \tag{18}$$

$$= (-1)^K \frac{2^{2K-1} \pi^{2K}}{(2K)!} B_{2K}\left(\frac{x+\pi}{2\pi}\right) \tag{19}$$

Fig. 1 illustrates a point emphasized by Lyness [34], which is that the FACE is usually an *asymptotic* but *divergent* expansion. The function $\hat{f}(x)$ in this example is generated by periodizing a function $f(x)$ which is analytic everywhere except for singularities outside $x \in [-\pi, \pi]$. The coefficients in the FACE show the factorial growth with order which is typical of divergent asymptotic series:

Table 1
Lanczos–Krylov functions that are Bernoulli polynomials.

$\mathcal{S}_1(x)$	$= \sum_{j=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin(nx)$ $= x/2$
$\mathcal{C}_2(x)$	$= \sum_{j=1}^{\infty} \frac{(-1)^{n+1}}{n^2} \cos(nx)$ $= -\frac{1}{4}x^2 + \frac{\pi^2}{12}$
$\mathcal{S}_3(x)$	$= \sum_{j=1}^{\infty} \frac{(-1)^{n+1}}{n^3} \sin(nx)$ $= -\frac{1}{12}x^3 + \frac{\pi^2}{12}x$
$\mathcal{C}_4(x)$	$= \sum_{j=1}^{\infty} \frac{(-1)^{n+1}}{n^4} \cos(nx)$ $= \frac{1}{48}x^4 - \frac{\pi^2}{24}x^2 + \frac{7\pi^4}{720}$

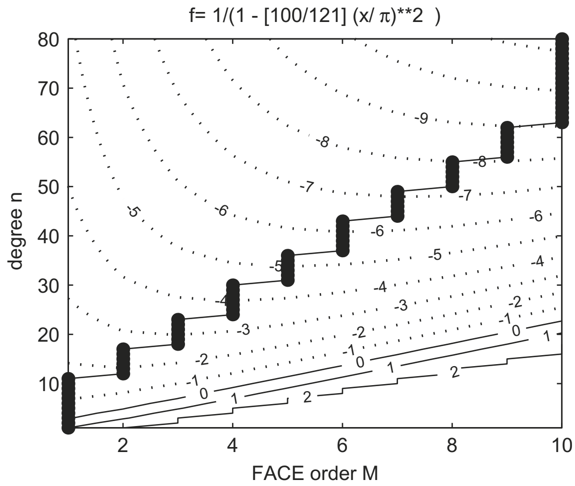

Fig. 1. Isolines of the base-10 logarithm of the error in approximating the n-th cosine coefficient by the Fourier Coefficient Asymptotic Approximation of a piecewise analytic function, $f(x) = 1/(1-(100/[121\pi^2])x^2$. The thick black curve with disks shows the optimum truncation order $m(n)$ of the series for a_n where "optimal" means that the expansion up to including n^{2m} gives the smallest error in approximating a_n for that value of n.

$$f(x) \equiv \frac{1}{1-0.826x^2/\pi^2} \Rightarrow a_n \sim -11.12/n^2 + 677.5/n^4 - 1.373E5/n^6 + 5.843E7/n^8 - 4.262E10/n^{10} + 4.751E13/n^{12} - 7.509E16/n^{14} + 1.598E20/n^{16} - 4.403E23/n^{18} + \dots \quad (20)$$

For fixed n, the error in approximating a_n by an inverse power series of the form of (2), truncated at the M-th term,

$$a_n \sim (-1)^{n+1} \sum_{k=1}^{M} \xi_k n^{-k} \quad (21)$$

decreases with increasing M, reaches a minimum at the "optimal truncation", $M = M_{opt}$, and then diverges to ∞ as $M \to \infty$. In the different limit that $n \to \infty$ for a fixed number of terms M in the asymptotic series, $\hat{f}(x)$, however, the error in approximating the Fourier coefficients by the FACE falls as $O(n^{2M+2})$. Equivalently, the error in approximating $\hat{f}(x)$ by a fixed sum of $\mathcal{C}_k(x)$ falls at the same rate over the entire interval.

3. How to compute the Lanczos–Krylov functions which are not Bernoulli polynomials (Clausen functions)

The non-polynomial LK functions are known also as the "Clausen functions" defined by

$$\mathcal{C}_{2m+1}(x) = -\mathrm{Cl}_{2m+1}(x+\pi), \quad \mathcal{S}_{2m}(x) = \mathrm{Cl}_{2m}(x+\pi), \quad (22)$$

where the definitions are those of Linton and Thompson [33].

The lowest non-Bernoulli LK function is given by the explicit formula

$$\mathcal{C}_1(x) = \sum_{j=1}^{\infty} \frac{(-1)^{n+1}}{n} \cos(nx) = \log\{2\cos(x/2)\} - \pi \leqslant x \leqslant \pi \quad (23)$$

The next Clausen function is

$$\mathcal{S}_2(x) \equiv \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n^2} \sin(nx) = \int_0^x \mathcal{C}_1(y)dy = \int_0^x \log(2\cos(y/2))dy \quad (24)$$

as follows by-term-by-term integration of the cosine series for $\mathcal{C}_1$. Unfortunately, this integral cannot be done in closed form.

Fortunately, the integrand does have the rapidly convergent expansion

$$\log(2\cos(y/2)) = \log(\pi - y) + \sum_{j=1}^{\infty} q_j (y-\pi)^{2j} \quad (25)$$

which can be obtained in the Maple symbolic language package by the line $y := w + Pi$; $J := 12$; $ls :=$ series(log(2 ∗ cos(y/2)), $w, 2 * J + 1$); or by the analytic formula

$$q_j = (-1)^j \frac{B_{2j}}{2j(2j)!}, \quad j = 1, 2, \dots \quad (26)$$

Because the function $\log(2\cos(y/2))$ has singularities at $\pm(2m+1)\pi$ for all integers m, it follows that the radius of convergence of the expansion about $y=\pi$ is 2π. Because the convergence-limiting singularity is a logarithm, it follows that the series coefficients are asymptotically proportional to, noting the q_j is the coefficient of the square of the j-th power of $(y-\pi)$, those of a logarithmic series with a radius of convergence of 2π, that is,

$$q_j \sim Q(2\pi)^{-2j}/j \tag{27}$$

where Q is a constant. This is confirmed in Table 2, which gives the coefficients themselves and also shows (in the rightmost table) that the proportionality constant Q is one.

We can numerically integrate this series term-by-term to approximate $\mathcal{S}_2$. Because all the LK functions have definite parity, that is,

$$\mathcal{S}_k(-x) = -\mathcal{S}_k(x), \quad \mathcal{C}_k(-x) = \mathcal{C}_k(x) \tag{28}$$

it is only necessary to apply the term-by-term integration on the restricted interval $x \in [0,\pi]$ because the LK functions can be evaluated for negative x by computing them for positive x and then applying the parity identities (28). It follows that the series at worst must be used a distance π from the expansion point. Truncating the series after the J-th term, the first neglected term at worst is about $4^{-(J+1)}/(J+1)$. If we stop after $J=12$, the highest term listed in the table, then the first neglected coefficient has a magnitude of only 1.1×10^{-9}. The error in the *integrated* series is even smaller.

Non-Bernoulli functions of higher k can be obtained by repeated integration. One complication is that each integration adds another constant of integration; $\mathcal{S}_4(x)$ is only determined to within the addition of an arbitrary quadratic polynomial, for example. However, symmetry with respect to the origin implies that the arbitrary polynomial in the $\mathcal{S}_k(x)$ must contain only *odd* powers of x while $\mathcal{C}_k(x)$ must have a polynomial part with only even powers. The coefficients of these polynomials of integration may be determined by summing the Fourier series and/or derivatives of the Fourier series to obtain the necessary boundary conditions at $x=0$ and $x=\pi$. For example, we first constructed the double integral of $\log(\pi-x)$ so that the resulting combination of logarithms and polynomial was zero at the origin, and then added the constant $\sum_{n=1}^{\infty}(-1)^{n+1}/n^3 = (3/4)\zeta(3) = 0.90154267736969572$, which is the value of $\mathcal{C}_3(0)$ (Table 3).

Table 2
Coefficients for $\log(2\cos(y/2))$.

j	q_j (exact)	q_j (floating point)	$q_j 4^j \pi^j j$
1	−1/24	−0.4166666666666667e−1	−1.644934
2	−1/2880	−0.3472222222222222e−3	−1.082323
3	−1/181440	−0.5511463844797178e−5	−1.017343
4	−1/9676800	−0.1033399470899471e−6	−1.004077
5	−1/479001600	−0.2087675698786810e−8	−1.000995
6	−691/15692092416000	−0.4403491782239578e−10	−1.000246
7	−1/1046139494400	−0.9558954664774771e−12	−1.000061
8	−3617/170729965486080000	−0.2118550185201614e−13	−1.000015
9	−43867/91963695909076992000	−0.4770034475709914e−15	−1.000004
10	−174611/16057153253965824000000	−0.1087434349279031e−16	−1.000001
11	−77683/310224200866619719680000	−0.2504092194709195e−18	−1.000000
12	−236364091/40651779281561848066867200000	−0.5814360285755218e−20	−1.000000

Table 3
Non-Bernoulli Lanczos–Krylov functions ("Clausen functions").

$\mathcal{C}_1(x)$	$=\sum_{j=1}^{\infty}\frac{(-1)^{n+1}}{n}\cos(nx)$
	$=\log\{2\cos(x/2)\}$
$\mathcal{S}_2(x)$	$=\sum_{j=1}^{\infty}\frac{(-1)^{n+1}}{n^2}\sin(nx)$
	$\times\ \pi\log(\pi)-x+(x-\pi)\log(\pi-x)+\sum_{j=1}^{\infty}q_j\{(x-\pi)^{2j+1}-(-\pi)^{2j+1}\}/(2j+1)$
	$=-\mathcal{S}_2(-x),\ x<0$
$\mathcal{C}_3(x)$	$=\sum_{j=1}^{\infty}\frac{(-1)^{n+1}}{n^3}\cos(nx)$
	$\times\ x^2\{\frac{3}{4}-\frac{1}{2}\log(\pi-x)\}+x\{\pi\log(\pi-x)-\frac{3}{2}\pi\}+\frac{\pi^2}{2}\{\log(\pi)-\log(\pi-x)\}+0.90154267736969572$
	$-\sum_{j=1}^{\infty}q_j\{(x-\pi)^{2j+2}-(-\pi)^{2j+2}\}/[(2j+1)(2j+2)]$
	$=\mathcal{C}_3(x),\ x<0$
$\mathcal{S}_4(x)$	$=\sum_{j=1}^{\infty}\frac{(-1)^{n+1}}{n^4}\sin(nx)$
	$\times\ \{\frac{11}{36}-\frac{1}{6}\log(\pi-x)\}x^3+\{\frac{\pi}{2}\log(\pi-x)-\frac{11\pi}{12}\}x^2+\left\{\frac{\pi^2}{36}(7+6\log(\pi))+\frac{5\pi^2}{12}-\frac{\pi^2}{2}\log(\pi-x)\right\}x$
	$+\frac{\pi^3}{6}(\log(\pi-x)-\log(\pi))-0.06934963385x$
	$-\sum_{j=1}^{\infty}q_j\{(x-\pi)^{2j+3}-(-\pi)^{2j+3}\}/[(2j+1)(2j+2)(2j+3)]$
	$=-\mathcal{S}_4(-x),\ x<0$

4. An example: $\sum_{n=1}^{\infty}(\pm 1)^{n+1}(1/(n+\lambda))\cos(nx)$

The function

$$\chi(x;\lambda) \equiv \sum_{n=1}^{\infty}(-1)^{n+1}\frac{1}{n+\lambda}\cos(nx) \tag{29}$$

arises in physics [40]. Oleksy obtained good results even very close to the singularity by performing a series of exact trigonometric transformations to create a sequence of new sums whose arguments $z(x)$ are much farther from the singularity than the argument x of the original series [40]. However, Oleksy's method does not explicitly display the singularities as done here.

Dillman and Grabitz [15], in treating Fourier–Bessel series for supersonic nozzle jets in fluid mechanics by "Kummer's method", were required to evaluate $\chi(x;\lambda)$ for reasons similar to our LK functions here. They note that $\chi(x;\lambda) = \Re(\Phi(\exp(ix);1,\lambda))$ where Φ is the "Lerch transcendent":

$$\Phi(z;s,a) \equiv \sum_{n=0}^{\infty}\frac{z^n}{(n+a)^s}, \quad |z|<1, \quad a \neq -1,-2,\ldots \tag{30}$$

By using identities for the Lerch transcendent, Dillman and Grabitz were able to evaluate the sum explicitly, but only for the special cases of $\lambda = 1/4$ and $\lambda = 3/4$.

To apply the LK functions to the series (29), note that

$$\frac{1}{n+\lambda} = \frac{1}{n}\frac{1}{1+\lambda/n} = \sum_{k=1}^{\infty}(-1)^{k-1}\lambda^{k-1}\frac{1}{n^k}, \tag{31}$$

Then (6) becomes

$$\chi(x;\lambda) = s_M + \sum_{k=1}^{\infty}(-\lambda)^{k-1}\{\mathcal{C}_k(x) - \mathcal{C}_{k,M}(x)\} \tag{32}$$

where $s_M = \sum_{n=1}^{M}(\pm 1)^{n+1}(1/(n+\lambda))\cos(nx)$. Fig. 2 shows a typical example. Since exact values for $\chi(x;\lambda)$ are not known, we summed 2000 terms using the x-dependent linear erfclog filter of [11] as the "benchmark". The difference between the benchmark and the LK sum is less than 10^{-10} over most of the interval.

There is a narrow zone near $x=\pi$ where the difference is large. This is not a fault of the LK method, but rather of the direct summation. The function $\chi(x;\lambda)$ has logarithmic singularities at $x = \pm\pi$. The direct sum, even with the use of a filter, cannot approximate the infinity at $x=\pi$. A logarithmic singularity is Gibbs Phenomenon with a vengeance! Even when the singularity is merely a discontinuity, all filters fail sufficiently close to the singularity [45,46].

In contrast, the leading logarithmic singularity is captured by $\mathcal{C}_1(x) = \log(2\cos(x/2))$ in the LK series, and weaker singularities proportional to $(\pi - x)^{k-1}\log(\pi - x)$ are displayed with the correct multipliers by the higher $\mathcal{C}_k(x)$ terms. Indeed, the LK decomposition is not merely a way to numerically evaluate the series, but also is a means to *classify* and *display* the type of singularity.

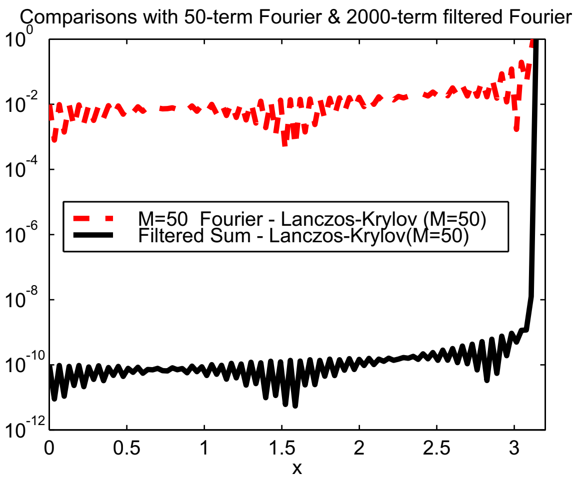

Fig. 2. Difference between $\chi(x;\lambda)$ for $\lambda = 1/2$ and the LK method using LK functions up to and including $\mathcal{C}_4(x)$ with the direct summation limit $M = 50$. The spike in the difference at $x = \pi$ is due to the failure of the filter near the logarithmic singularity of $\chi(x;\lambda)$; the LK method is accurate for all x.

5. Summary and extensions

The Lanczos–Krylov singularity subtraction method [20] is restricted to piecewise analytic functions. Our procedure is broader because it can cope with logarithmic endpoint singularities, too. Our example is one such function that has arisen in physics. Most prior work has focused on using either discrete samples of $f(x)$ or the analytical form of the function to deduce the terms in the Fourier coefficient asymptotic approximation. Here, we have assumed that an analytical form for the Fourier coefficients is already known, and devised a summation method that proceeds from this starting point.

Several obvious extensions are possible. If only numerical values for the Fourier coefficients are known, instead of an analytic formula, interpolation of the coefficients in powers of $1/n$ can supply the coefficients ξ_k in (2).

A differential equation such as

$$u_{xx} - u = -f(x), \quad u(0) = u(\pi) \tag{33}$$

can be easily solved in series form by writing

$$f(x) = \sum_{n=1}^{\infty} f_n \sin(nx) \to u(x) = \sum_{n=1}^{\infty} \frac{f_n}{1+n^2} \sin(nx) \tag{34}$$

Unfortunately, if $f(x)$ is not a periodic function, then its Fourier series will converge as $O(1/n)$, which removes much of the charm from what otherwise is an appealingly simple strategy. However, the Fourier coefficient asymptotic expansion (15), together with a geometric expansion of $(1/(1+n^2)$ will furnish an approximation of the sine coefficients of $u(x)$ in powers of $1/n$, and then the LK series can be applied. For example, if $f(x) = x \to f_n = 2(-1)^{n+1}/n$, one finds that

$$u(x) = \sum_{n=1}^{M} \left\{ \frac{2(-1)^{n+1}}{n(1+n^2)} - 2(-1)^{n+1} \sum_{k=1}^{K} (-1)^{k-1} \frac{1}{n^{2k+1}} \right\} \sin(nx) + 2\sum_{k=1}^{K} (-1)^{k-1} \mathcal{S}_{2k+1}(x) + O\left(\frac{1}{(M+1)^{2K+3}} \right) \tag{35}$$

The principle is the same when $f(x)$ has a more complicated sine expansion.

The Lanczos–Krylov decomposition, even as generalized here, is not directly applicable to a Fourier series such as

$$\sigma(x) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\log(n)}{1+n^2} \cos(nx) \tag{36}$$

The logarithm in the Fourier coefficient implies that the singularity of $\sigma(x)$ at $x = \pm\pi$ is more complicated than a simple derivative discontinuity or $\log(x)$. However, if one can find a closed form solution for the simpler series $\sum_{n=1}^{\infty} (-1)^{n+1} \frac{\log(n)}{n^{2k}} \cos(nx)$, then one can define a new set of LK functions for this type of singularity, and the rest goes as before [8].

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References

[1] R. Archibald, K.W. Chen, A. Gelb, R. Renaut, Improving tissue segmentation of human brain MRI through preprocessing by the Gegenbauer reconstruction method, Neuroimage 20 (2003) 489–502.
[2] R. Archibald, A. Gelb, A method to reduce the Gibbs ringing artifact in MRI scans while keeping tissue boundary integrity, IEEE Trans. Med. Imaging 21 (2002) 305–319.
[3] R. Archibald, A. Gelb, J.H. Yoon, Polynomial fitting for edge detection in irregularly sampled signals and images, SIAM J. Numer. Anal. 43 (2005) 259–279.
[4] R. Archibald, J.X. Hu, A. Gelb, G. Farin, Improving the accuracy of volumetric segmentation using pre-processing boundary detection and image reconstruction, IEEE Trans. Image Process. 13 (2004) 459–466.
[5] G. Baszenski, F. Delvos, Error estimates for sine series expansions, Mathematische Nachrichten 139 (1988) 155–166.
[6] G. Baszenski, F.-J. Delvos, M. Tasche, A unified approach to accelerating trigonometric expansions, Comput. Math. Appl. 30 (1995) 33–49.
[7] S. Biringen, K.H. Kao, On the application of pseudospectral FFT techniques to nonperiodic problems, Internat. J. Numer. Fluids 9 (1989) 1235–1267.
[8] J.P. Boyd, The asymptotic Chebyshev coefficients for functions with logarithmic endpoint singularities, Appl. Math. Comput. 29 (1989) 49–67.
[9] Sum-accelerated pseudospectral methods: The Euler-accelerated sinc algorithm, App. Numer. Math. 7 (1991) 287–296.
[10] A lag-averaged generalization of Euler's method for accelerating series, Appl. Math. Comput. 72 (1995) 146–166.
[11] The Erfc-Log filter and the asymptotics of the Vandeven and Euler sequence accelerations, in: A.V. Ilin, L.R. Scott (Eds.), Proceedings of the Third International Conference on Spectral and High Order Methods, Houston, Texas, 1996, Houston Journal of Mathematics, pp. 267–276.
[12] Two comments on filtering, J. Comput. Phys. 143 (1998) 283–288.
[13] Chebyshev and Fourier Spectral Methods, Dover, New York, 2001.
[14] J.P. Boyd, D.W. Moore, Summability methods for Hermite functions, Dyn. Atmos. Oceans 10 (1986) 51–62.
[15] A. Dillmann, G. Grabitz, On a method to evaluate Fourier–Bessel series with poor convergence properties and its application to linearized supersonic free jet flow, Quart. J. Appl. Math. 53 (1995) 335–352.
[16] T.A. Driscoll, B. Fornberg, A Padé-based algorithm for overcoming the Gibbs phenomenon, Numer. Algorithms 26 (2001) 77–92.
[17] K.S. Eckhoff, On discontinuous solutions of hyperbolic equations, in: C. Bernardi, Y. Maday (Eds.), Analysis, algorithms and applications of spectral and high order methods for partial differential equations, selected papers from the international conference on spectral and high order methods (ICOSAHOM'92), Le Corum, Montpellier, France, 22–26 June 1992, North-Holland, Amsterdam, 1994, 103–112. Also in Comput. Meth. Appl. Mech. Engrg., 116.
[18] Accurate reconstructions of functions of finite regularity from truncated Fourier series expansions, Math. Comput., 64 (1995) 671–690.

[19] On a high order numerical method for solving partial differential equations in complex geometries, J. Sci. Comput., 12 (1997) 119–138.
[20] On a high order numerical method for functions with singularities, Math. Comput. 67 (1998) 1063–1087.
[21] J. Geer, N.S. Banerjee, Exponentially accurate approximations to piece-wise smooth periodic functions, J. Sci. Comput. 12 (1997) 253–287.
[22] A. Gelb, E. Tadmor, Spectral reconstruction of piecewise smooth functions from their discrete data, Model. Math. Anal. Numer. 36 (2002) 155–175.
[23] D. Gottlieb, C.-W. Shu, On the Gibbs phenomenon and its resolution, SIAM Rev. 39 (1997) 644–668.
[24] D. Gottlieb, C.-W. Shu, A. Solomonoff, H. Vandeven, On the Gibbs phenomenon I: recovering exponential accuracy from the Fourier partial sum of a nonperiodic analytic function, J. Comput. Appl. Math. 43 (1992) 81–98.
[25] A.J. Jerri (Ed.), Gibbs Phenomenon, Sampling Publishing, Potsdam, NY, 2008, p. 500.
[26] J. Jung, B.D. Shizgal, Generalization of the inverse polynomial reconstruction method in the resolution of the Gibbs phenomenon, J. Comput. Appl. Math. 172 (2004) 131–151.
[27] Inverse polynomial reconstruction method in the resolution of the Gibbs phenomenon, J. Sci. Comput. 25 (2005) 367–399.
[28] J. Jung, B.D. Shizgal, On the numerical convergence with the inverse polynomial reconstruction method for the resolution of the Gibbs phenomenon, J. Comput. Phys. 224 (2007) 477–488.
[29] G. Kvernadze, Determination of the jumps of a bounded function by its Fourier series, J. Approx. Theory 92 (1998) 167–190.
[30] G. Kvernadze, T. Hagstrom, H. Shapiro, Detecting the singularities of a function of vp class by its integrated Fourier series, Comput. Math. Appl. 39 (2000) 301.
[31] C. Lanczos, Evaluation of noisy data, SIAM J. Numer. Anal. 1 (1964) 76–85.
[32] Discourse on Fourier Series, Oliver and Boyd, Edinburgh, 1966.
[33] C.M. Linton, I. Thompson, One- and two-dimensional lattice sums for the threedimensional Helmholtz equation, J. Comput. Phys. in press.
[34] J.N. Lyness, Computational techniques based on the Lanczos representation, Math. Comput. 28 (1974) 81–123.
[35] The calculation of trigonometric Fourier coefficients, J. Comput. Phys. 54 (1984) 57–73.
[36] A. Majda, J. McDonough, S. Osher, The Fourier method for nonsmooth initial data, Math. Comput. 32 (1978) 1041–1081.
[37] S.L. Marshall, Convergence acceleration of Fourier series by analytical and numerical application of Poisson's formula, J. Phys. A 31 (1998) 2691–2704.
[38] On the analytical summation of Fourier series and its relation to the asymptotic behavior of Fourier transforms, J. Phys. A 31 (1998) 9957–9973.
[39] A. Nersessian, A. Poghosyan, On a rational linear approximation of Fourier series for smooth functions, J. Sci. Comput. 26 (2006) 111–125.
[40] C. Oleksy, A convergence acceleration method of Fourier series, Comput. Phys. Commun. 96 (1996) 17–26.
[41] S. Paszkowski, Convergence acceleration of orthogonal series, Numer. Algorithms 47 (2008) 35–62.
[42] P.J. Roache, A pseudo-spectral FFT technique for non-periodic problems, J. Comput. Phys. 27 (1978) 204–220.
[43] E. Tadmor, J. Tanner, Adaptive mollifiers for high resolution recovery of piecewise smooth data from its spectral information, Foundations Comput. Math. 2 (2002) 155–189.
[44] Adaptive filters for piecewise smooth spectral data, IMA J. Numer. Anal. 25 (2005) 635–647.
[45] J. Tanner, Optimal filter and mollifier for piecewise smooth spectral data, Math. Comput. 75 (2006) 767–790.
[46] H. Vandeven, Family of spectral filters for discontinuous problems, J. Sci. Comput. 6 (1991) 159–192.
[47] L. Vozovoi, M. Israeli, A. Averbuch, Analysis and application of the Fourier–Gegenbauer method to stiff differential equations, SIAM J. Numer. Anal. 33 (1996) 1844–1863.
[48] L. Vozovoi, A. Weill, M. Israeli, Spectrally accurate solution of non-periodic differential equations by the Fourier–Gegenbauer method, SIAM J. Numer. Anal. 34 (1997) 1451–1471.
[49] H. Wengle, J.H. Seinfeld, Pseudospectral solution of atmospheric diffusion problems, J. Comput. Phys. 26 (1978) 87–106.
[50] R.K. Wright, A robust method for accurately representing nonperiodic functions given Fourier coefficient information, J. Comput. Appl. Math. 140 (2002) 837–848.
[51] Local spline approximation of discontinuous functions and location of discontinuities, given low-order Fourier coefficient information, J. Comput. Appl. Math. 164–165 (2004) 783–795.