From high oscillation to rapid approximation I: Modified Fourier expansions

Arieh Iserles
DAMTP, Centre for Mathematical Sciences
University of Cambridge
Wilberforce Rd, Cambridge CB3 0WA
United Kingdom

Syvert P. Nørsett
Department of Mathematics
Norwegian University of Science and Technology
Trondheim N-7491
Norway

June 20, 2006

Abstract

In this paper we consider a modification of the classical Fourier expansion, whereby in $[-1, 1]$ the $\sin \pi nx$ functions are replaced by $\sin \pi(n - \frac{1}{2})x$, $n \geq 1$. This has a number of important advantages in the approximation of analytic, nonperiodic functions. In particular, expansion coefficients decay like $\mathcal{O}\left(n^{-2}\right)$, rather than like $\mathcal{O}\left(n^{-1}\right)$.

We explore theoretical features of these *modified Fourier expansions*, prove suitable versions of Fejér and de la Vallée Poussin theorems and expand the coefficients into asymptotic series.

This expansion is a key toward the computation of expansion coefficients by asymptotic and Filon-type methods. We explore this issue in some detail and present a number of algorithms which require $\mathcal{O}(m)$ operations in the computation of the first m expansion coefficients.

1 Introduction

By any yardstick, Fourier series are one of the greatest and most influential concepts of contemporary mathematics. They have spawned an entire discipline, harmonic analysis, and their applications range widely, from number theory to electrical engineering, from theoretical computer science to signal and image processing (Körner 1988). The computation of Fourier coefficients by means of the discrete Fourier transform and its numerical manifestation, the Fast Fourier Transform (FFT), literally transformed modern technology and science and informed much of modern numerical analysis (Henrici 1986). Arguably, the FFT is the most influential computational algorithm ever. It is thus with a measure of trepidation and humility that we wish to pursue an alternative approach in this paper.

The standard setting of Fourier analysis, which plays to its strengths, is when f is analytic in an open set containing $[-1,1]$ and periodic with period 2. (We could have replaced $[-1,1]$ by an arbitrary compact interval.) In that case Fourier expansion enjoys three crucial advantages:

1. The Fourier expansion of f is
$$\sum_{n=-\infty}^{\infty} \hat{f}_n \mathrm{e}^{\mathrm{i}n\pi x}, \tag{1.1}$$
where
$$\hat{f}_n = \int_{-1}^{1} f(x)\mathrm{e}^{-\mathrm{i}\pi n x}\mathrm{d}x, \qquad n \in \mathbb{Z}.$$
The expansion (1.1) converges to f pointwise in $[-1,1]$ and this process is very rapid indeed: there exist $c > 0$ and $\alpha > 0$ such that $|\hat{f}_n| \le c\mathrm{e}^{-\alpha n}$ for all $n \in \mathbb{Z}$.

2. Once the integral is replaced by a finite sum,
$$\hat{f}_n \approx \hat{F}_{n,m} = \frac{1}{m}\sum_{k=0}^{m-1} f(\tfrac{k}{m}) \exp\left(-\frac{\mathrm{i}\pi n k}{m}\right), \tag{1.2}$$
we commit exponentially small error, $|\hat{F}_{n,m} - \hat{f}_n| \le c_1 \mathrm{e}^{-\alpha m}$.

3. Suppose that m is a highly-composite integer: to all intents and purposes, we may assume that $m = 2^r$ for some $r \ge 1$. The *Discrete Fourier Transform (DFT)* $\mathcal{F}_m[f] = \{\hat{F}_{n,m}\}_{n=-m/2+1}^{m/2}$ can be computed in $\mathcal{O}(m \log_2 m)$ operations using FFT (Henrici 1986).

In their totality, these three features account for the phenomenal success of Fourier expansions in a wide range of applications. Yet, this success looses much of its lustre once f is not a periodic function. Specifically,

1. Although (1.1) is pointwise convergent to f at all points of analyticity (thus, in $(-1,1)$, but not at the endpoints), the coefficients decay very slowly indeed: $|\hat{f}_n| = \mathcal{O}\big(n^{-1}\big)$, $n \gg 1$.

2. Quadrature (1.2) produces *much* larger error: $|\hat{F}_{n,m} - \hat{f}_n| \le c_2/m^2$.

Once exponential convergence and exponentially-fast decay of the error are no longer valid, Fourier expansion becomes less attractive. This might account for the ubiquity of periodic boundary conditions in applications, a phenomenon not always justified by the underlying physical model. This also explains the great deal of attention paid to the *Gibbs phenomenon* and computational devices for its treatment throughout numerical and engineering literature.

Matters are considerably worse when f is just an $\mathrm{L}_2[-1,1]$ function, but we do not intend to dwell on this issue. Analyticity makes for the simplest and clearest framework to present the arguments of this paper, while virtually all of our work generalises to $\mathrm{C}^r[-1,1]$ functions for suitable $r \in \mathbb{N}$ in a fairly transparent manner.

Fast Fourier Transform, its many successes notwithstanding, also exhibits a built-in inefficiency: it is not very adaptive. Suppose, thus, the we wish to approximate $\hat{f}_n$, $-m/2+1 \le n \le m/2$, by FFT. How to choose m? If it is too large, we clearly pay a price, e.g. in function evaluations or (for example, in spectral methods) size of an algebraic linear system that we must solve. If it is too small, though, we need to increase it to the next highly-composite integer (in the simplest implementation, double it), while discarding our computations. In an ideal world, we would have liked an efficient algorithm that produces Fourier components consecutively, until we decide that we have had enough. Of course, once f is analytic and periodic, lack of adaptivity is more than offset by the extraordinary precision and speed of FFT, but this need not be so once periodicity is lost.

Our proposed modification to the Fourier setting is, on the face of it, quite minor. We commence by rewriting (1.1) in the form

$$\tfrac{1}{2}\hat{f}_0^C + \sum_{n=1}^{\infty}[\hat{f}_n^C \cos\pi nx + \hat{f}_n^D \sin\pi nx],$$

where

$$\hat{f}_n^C = \int_{-1}^{1} f(x)\cos\pi nx\,\mathrm{d}x, \qquad \hat{f}_n^D = \int_{-1}^{1} f(x)\sin\pi nx\,\mathrm{d}x.$$

We propose to replace $\sin\pi nx$ by $\sin\pi(n-\frac{1}{2})x$, $n\in\mathbb{N}$ and consider the *modified Fourier expansion*

$$\tfrac{1}{2}\hat{f}_0^C + \sum_{n=1}^{\infty}[\hat{f}_n^C \cos\pi nx + \hat{f}_n^S \sin\pi(n-\tfrac{1}{2})x], \qquad (1.3)$$

where $\hat{f}_n^C$ remains unamended, while

$$\hat{f}_n^S = \int_{-1}^{1} f(x)\sin\pi(n-\tfrac{1}{2})x\,\mathrm{d}x.$$

In the sequel, we intend to prove the following features of the modified Fourier expansion.

a. The set
$$\mathcal{H}_1 = \{\cos\pi nx \,:\, n\in\mathbb{Z}_+\} \cup \{\sin\pi(n-\tfrac{1}{2})x \,:\, n\in\mathbb{N}\}$$
consists of orthogonal functions and it is dense in $\mathrm{L}_2[-1,1]$;

b. Suitably amended, the classical Fejér and de la Vallée Poussin theorems remain valid in this setting and ensure pointwise convergence subject to fairly general conditions.

c. So far, we have seen that (1.3) shares some of the features of the classical Fourier expansion (1.1). It is central to our interest in modified Fourier expansion that it exhibits superior behaviour once analytic f is no longer periodic. At the first instance we note faster convergence: specifically, $|\hat{f}_n^C|, |\hat{f}_n^S| = \mathcal{O}(n^{-2})$ for $n \gg 1$.

d. Instead of approximating Fourier coefficients by the Discrete Fourier Transform (1.2) (or by Discrete Cosine and Sine Transforms (Rao & Yip 1990)), we expand them into asymptotic series. This allows for a computation of each coefficient, up to accuracy $\mathcal{O}(n^{-2r-2})$ for some $r\in\mathbb{N}$, in a constant number of operations. Thus, we can compute $\hat{f}_n^C$ and $\hat{f}_n^S$ to suitably high precision for $n \le m$ in $\mathcal{O}(m)$ operations.

e. Computation of Fourier coefficients can be further improved, increasing precision and reducing cost, once we employ techniques for the computation of highly oscillatory integrals introduced by the current authors in (Iserles & Nørsett 2004, Iserles & Nørsett 2005) and based on Filon-type quadrature.

To our knowledge, the basis $\mathcal{H}_1$ has been originally proposed by Mark Krein in his investigation of differential operators (Krein 1935). It also features in nonharmonic Fourier analysis, in particular in the proof of the Kadec $\frac{1}{4}$-theorem (Young 1980). However, as far as we are aware, it has never been analysed in depth or employed as a practical means to approximate functions.

A replacement of the classical Fourier expansion (1.1) by its modification (1.3) is just a first step in a longer journey toward a theory of rapid approximation of functions. Once the mechanism underlying the increase in the rate of convergence in (1.3) is understood, it is possible to generalise it. The outcome is a hierarchy of approximation bases $\mathcal{H}_s$ such that each $\mathcal{H}_s$ approximates analytic functions in $[-1,1]$ at a rate of $\mathcal{O}(n^{-s-1})$. All such bases can be constructed explicitly. Moreover, the first m expansion coefficients can be approximated to high precision in $\mathcal{O}(m)$ operations, employing again asymptotic and Filon-type techniques. This will be a subject of a forthcoming paper. Another forthcoming paper will address itself to the challenge of extending our framework to multivariate setting. Unlike the classical Fourier approach of Cartesian products, which is valid only in parallelepipeds, we devise a theory allowing for rapid approximation tailored to general bounded domains in $\mathbb{R}^d$.

2 The theory of modified Fourier expansions

It is instructive to commence our analysis from a numerical example. In Fig. 2.1 we display pointwise errors generated by classical and modified Fourier expansions of $f(x) = \mathrm{e}^x - \cosh(1)$ in the interval $[-\frac{9}{10}, \frac{9}{10}]$. Two observations stare us in the face. Firstly, modified Fourier expansion generates substantially smaller error. Secondly, once m, the number of harmonics, is doubled, the error of classical Fourier decreases by a factor of two (as predicted by general theory, (Körner 1988)), while the error of (1.3) goes down by a factor of four.

Fig. 2.1 stays clear from the endpoints, where classical Fourier expansion does not converge to f but to $\frac{1}{2}[f(-1)+f(1)]$. Modified Fourier converges to f, albeit slower than in $(-1,1)$. To explore this, we set

$$\mathcal{F}_m[f](x) = \tfrac{1}{2}\hat{f}_0^C + \sum_{n=1}^{m}[\hat{f}_n^C \cos \pi n x + \hat{f}_n^D \sin \pi n x],$$

$$\mathcal{M}_m[f](x) = \tfrac{1}{2}\hat{f}_0^C + \sum_{n=1}^{m}[\hat{f}_n^C \cos \pi n x + \hat{f}_n^S \sin \pi (n-\tfrac{1}{2}) x].$$

Fig. 2.2 displays (on the left) the *scaled* error $m|\mathcal{M}[f](1)-f(1)|$: it is clear that the (unscaled) error decays like $\mathcal{O}(m^{-1})$. The remainder of the figure revisits the case when $x \in (-1,1)$. Specifically, we let $x = \mathrm{e}^{-1}$ as a representative of $x \in (-1,1)$ and note from the scaling that, as we have already intimated, the errors for Fourier and modified Fourier decay like $\mathcal{O}(m^{-1})$ and $\mathcal{O}(m^{-2})$, respectively.

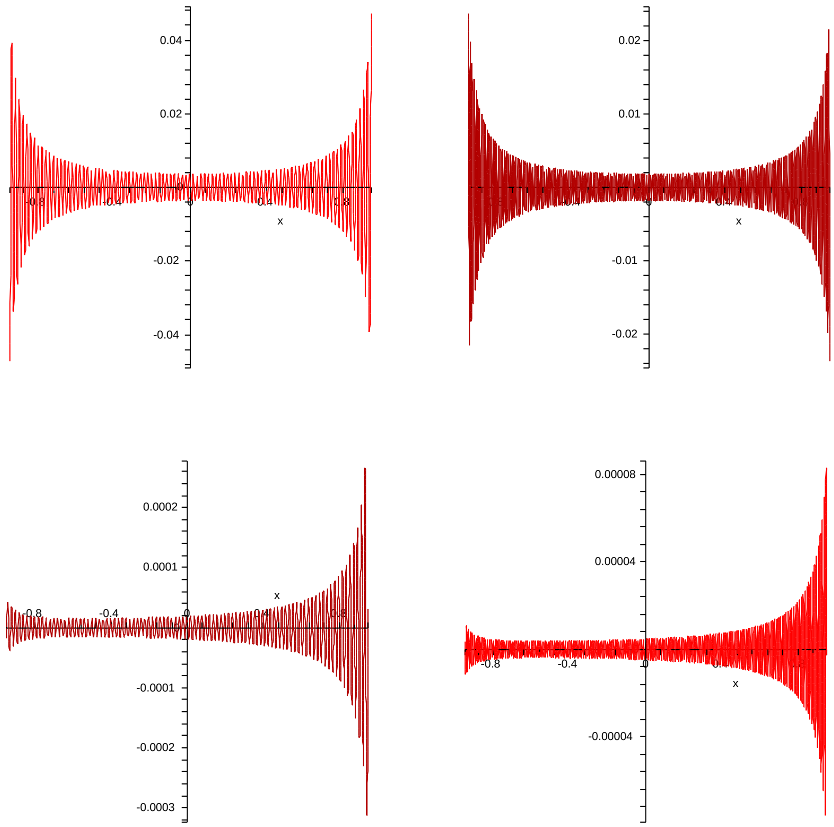

Figure 2.1: Absolute errors for Fourier (top row) and modified Fourier expansions of $f(x) = \mathrm{e}^x - \cosh(1)$ with $m = 100$ (left column) and $m = 200$ (right column).

The coefficients in the present case can be evaluated explicitly with great ease and they give the game away:

$$\hat{f}_n^C = \frac{2(-1)^n \sinh 1}{1 + \pi^2 n^2}, \qquad \hat{f}_n^D = \frac{2(-1)^{n+1} n\pi \sinh 1}{1 + \pi^2 n^2}, \qquad \hat{f}_n^S = \frac{2(-1)^{n+1} \cosh 1}{1 + \pi^2 (n - \frac{1}{2})^2}.$$

Thus, while $\hat{f}_n^D = \mathcal{O}(n^{-1})$, both $\hat{f}_n^C$ and $\hat{f}_n^S$ decay like $\mathcal{O}(n^{-2})$ for large n. We will see in the sequel that this is a demonstration of a more general pattern.

2.1 Convergence in $\mathrm{L}_2[-1, 1]$

The density of the set

$$\mathcal{H}_1 = \{\cos \pi n x \,:\, n \in \mathbb{Z}_+\} \cup \{\sin \pi (n - \tfrac{1}{2}) x \,:\, n \in \mathbb{N}\}$$

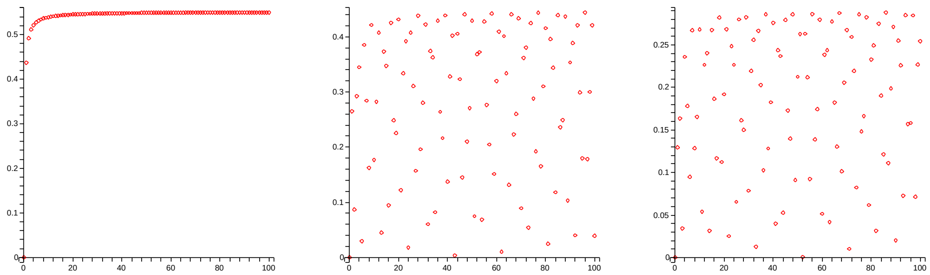

Figure 2.2: From left to right, scaled errors $m|\mathcal{M}_m[f](1) - f(1)|$, $m|\mathcal{F}_m[f](\mathrm{e}^{-1}) - f(\mathrm{e}^{-1})|$ and $m^2|\mathcal{M}_m[f](\mathrm{e}^{-1}) - f(\mathrm{e}^{-1})|$ respectively.

in $\mathrm{L}_2[-1,1]$ is embarrassingly easy to prove.

Theorem 1 *The set $\mathcal{H}$ is an orthonormal basis of* $\mathrm{L}_2[-1,1]$.

Proof We commence from the observation that $\cos \pi n x$, $n \in \mathbb{Z}_+$, and $\sin \pi(n - \frac{1}{2})x$, $n \in \mathbb{N}$, are all the eigenfunctions of the Sturm–Liouville operator $\mathcal{L} = \mathrm{d}^2/\mathrm{d}x^2$ with the Neumann boundary conditions $u'(-1) = u'(1) = 0$. (The corresponding eigenvalues are $-\pi^2 n^2$ and $-\pi^2(n - \frac{1}{2})^2$ respectively.) Both orthogonality and density in $\mathrm{L}_2[-1,1]$ follow at once from this observation using elementary spectral theory (Davies 1995), while the fact that all the terms in $\mathcal{H}_1$ share unit Euclidean norm can be confirmed by trivial integration. □

2.2 Asymptotic behaviour of the coefficients

A key feature of the technique proposed in this paper is that, once f is analytic, the coefficients of (1.3) exhibit relatively more rapid decay than those of the Fourier expansion (1.1). Moreover, our method of proof sets the stage for the development of computational techniques for rapid approximation of these coefficients.

Integrating the integral $\hat{f}_n^C$ by parts twice leads at once to the identity

$$\hat{f}_n^C = \frac{(-1)^n}{n^2\pi^2}[f'(1) - f'(-1)] - \frac{1}{n^2\pi^2}\int_{-1}^{1} f''(x)\cos \pi n x \mathrm{d}x.$$

Identifying the integral on the right as a "Fourier-cosine" coefficient of f'' and iterating this expression, we have

$$\hat{f}_n^C = \frac{(-1)^n}{(n\pi)^2}[f'(1) - f'(-1)] - \frac{(-1)^n}{(n\pi)^4}[f'''(1) - f'''(-1)] + \frac{1}{(n\pi)^4}\int_{-1}^{1} f^{(\mathrm{iv})}(x)\cos n\pi x \mathrm{d}x$$

and, recurring further, it readily follows by induction that $\hat{f}_n^C$ can be expanded asymptotically in the form

$$\hat{f}_n^C \sim (-1)^n \sum_{k=0}^{\infty} \frac{(-1)^k}{(n\pi)^{2k+2}}[f^{(2k+1)}(1) - f^{(2k+1)}(-1)], \qquad n \gg 1. \tag{2.1}$$

We emphasize that (2.1) holds only in an asymptotic sense. In other words, for every $r \in \mathbb{Z}_+$ it is true that

$$\hat{f}_n^C = (-1)^n \sum_{k=0}^{r} \frac{(-1)^k}{(n\pi)^{2k+2}} [f^{(2k+1)}(1) - f^{(2k+1)}(-1)] + \mathcal{O}\big(n^{-2r-4}\big)$$

for $n \gg 1$. It certainly does not mean that the infinite series in (2.1) converges in a standard sense for fixed n. Note that the expansion (2.1) makes sense for analytic (or at the very least C^∞) functions, but can be extended, with obvious amendments, to C^r functions for sufficiently large r.

The most important observation from (2.1) is that $\hat{f}_n^C = \mathcal{O}\big(n^{-2}\big)$. Seemingly, this is at variance with our statement that classical Fourier coefficients for analytic (nonperiodic) functions decay like $\mathcal{O}\big(n^{-1}\big)$, but the contradiction is purely illusory. *The $\mathcal{O}\big(n^{-1}\big)$ rate of decay is exhibited by the "Fourier-sine" coefficients $\hat{f}_n^D$.* Specifically, proceeding as before, it is easy to confirm that

$$\hat{f}_n^D \sim (-1)^{n-1} \sum_{k=0}^{\infty} \frac{(-1)^k}{(n\pi)^{2k+1}} [f^{(2k)}(1) - f^{(2k)}(-1)], \qquad n \gg 1. \tag{2.2}$$

Incidentally, note that when f is periodic, the right-hand side of both (2.1) and (2.2) vanishes. In other words, both $\hat{f}_n^C$ and $\hat{f}_n^D$ decay in that case faster than $\mathcal{O}(n^{-s})$ for any $s \in \mathbb{N}$: this is fully consistent with exponential decay.

The slow rate of decay of the $\hat{f}_n^D$ coefficients is the prime motivation behind the replacement of $\sin \pi n x$ by $\sin \pi(n - \frac{1}{2})x$ in our basis. Specifically, revisiting the procedure that led to (2.1) and (2.2), we obtain

$$\hat{f}_n^S \sim (-1)^{n-1} \sum_{k=0}^{\infty} \frac{(-1)^k}{[(n-\frac{1}{2})\pi]^{2k+2}} [f^{(2k+1)}(1) + f^{(2k+1)}(-1)]. \tag{2.3}$$

Thus, $\hat{f}_n^S = \mathcal{O}\big(n^{-2}\big)$, explaining the superior behaviour of modified Fourier expansions, as observed in Figure 2.1.

Before we advance further and examine the behaviour of modified Fourier expansions in greater detail, we wish to address a well-known technique in computational Fourier analysis which accelerates the convergence of classical Fourier series, thereby being an apparent competitor of our approach. Given an analytic (or sufficiently smooth) function f, we write it in the form

$$f(x) = [f(x) - p(x)] + p(x), \tag{2.4}$$

where p is a polynomial of degree $4r+1$ such that $p^{(k)}(\pm 1) = f^{(k)}(\pm 1)$, $k = 0, 1, \ldots, 2r$ – such Hermite interpolation always exists and is unique. It now follows from (2.1) and (2.2) that the Fourier coefficients of $f - p$ decay like $\mathcal{O}\big(n^{-2r-2}\big)$. Since Fourier coefficients of p can be evaluated exactly with great ease, this is a powerful device to accelerate the convergence of classical Fourier series.

An identical device can be applied to the modified Fourier expansion (1.3), but with an important difference. Note from (2.1) and (2.3) that *both* $\hat{f}_n^C$ and $\hat{f}_n^S$ can be expanded asymptotically in *odd* derivatives of f. In other words, once we write f in the form (2.4), we need

p to interpolate just odd derivatives. In place of the 'full' interpolation conditions at the endpoints, we require

$$q^{(2k)}(\pm 1) = f^{(2k+1)}(\pm 1), \qquad k = 0, 1, \ldots, r-1, \tag{2.5}$$

and set $p(x) = f(0) + \int_0^x q(\xi)\mathrm{d}\xi$. Our contention is that the $2r$ conditions (2.5) are satisfied uniquely by an $(2r-1)$-degree polynomial, hence that we can take p as a polynomial of degree $2r$, half of that required in the classical Fourier case.

This is not a trivial statement, since (2.5) is a *Birkhoff–Hermite interpolation problem* (Lorenz, Jetter & Riemenschneider 1983) and *a priori* there is no certainty that it can be obeyed by an $(2r-1)$-degree polynomial. This, however, is easy to prove. We demonstrate this for $r = 3$ but a generalization for all $r \in \mathbb{N}$ is straightforward. Once we express q in terms of its coefficients, (2.5) for $r = 3$ becomes a linear system with the 6×6 matrix

$$\begin{bmatrix} 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 2 & -6 & 12 & -20 \\ 0 & 0 & 2 & 6 & 12 & 20 \\ 0 & 0 & 0 & 0 & 24 & -120 \\ 0 & 0 & 0 & 0 & 24 & 120 \end{bmatrix}.$$

We now replace every $(2i-1)$th and $(2i)$th row by half their sum and half their difference, respectively. Next, we arrange first the odd rows and columns, followed by even rows and columns. The outcome,

$$\left[\begin{array}{ccc|ccc} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 2 & 12 & 0 & 0 & 0 \\ 0 & 0 & 24 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 6 & 20 \\ 0 & 0 & 0 & 0 & 0 & 120 \end{array}\right],$$

is reducible to two 3×3 linear systems with nonsingular upper-triangular matrices. Therefore the matrix is nonsingular and (2.5) possesses a unique solution with an $(2r-1)$-degree polynomial q.

2.3 Pointwise summability and convergence

In this subsection we intend to generalize to the present setting two classical theorems of harmonic analysis: the Fejér theorem on summability of Fourier series and the de la Vallée Poussin theorem on their convergence (Körner 1988).

We commence by decomposing f into its even and odd parts, $f = f_e + f_o$, where

$$f_e(x) = \tfrac{1}{2}[f(x) + f(-x)], \qquad f_o = \tfrac{1}{2}[f(x) - f(-x)].$$

Since $\hat{f}_{on}^{C}, \hat{f}_{en}^{D}, \hat{f}_{en}^{S} \equiv 0$, we observe that classical and modified Fourier series are identical for f_e and the only discernible difference is in their treatment of the odd function f_o. Since Fejér and de la Vallée Poussin theorems are thus correct for f_e, we assume in this subsection without loss of generality that f is odd.

Given $m \in \mathbb{N}$, we let

$$S_m[f](x) = \sum_{n=1}^{m} \hat{f}_n^S \sin \pi(n - \tfrac{1}{2})x,$$
$$\sigma_m[f](x) = \frac{1}{m} \sum_{n=1}^{m} S_n[f](x)$$

(we reiterate that f is now odd, hence we need consider only the sine terms). Therefore,

$$\begin{aligned}\sigma_m[f](x) &= \frac{1}{m} \int_{-1}^{1} f(\xi) \sum_{n=1}^{m} (m-n+1) \sin \pi(n - \tfrac{1}{2})\xi \sin \pi(n - \tfrac{1}{2})x \mathrm{d}\xi \\ &= \frac{1}{2m} \int_{-1}^{1} f(\xi) \sum_{n=1}^{m} (m-n+1)[\cos \pi(n - \tfrac{1}{2})(x-\xi) - \cos \pi(n - \tfrac{1}{2})(x+\xi)] \mathrm{d}\xi.\end{aligned}$$

However,

$$\begin{aligned}\sum_{n=1}^{m} (m-n+1) \cos(n - \tfrac{1}{2})\alpha &= \operatorname{Re} \sum_{n=1}^{m} (m-n+1) \mathrm{e}^{\mathrm{i}(n-\frac{1}{2})\alpha} \\ &= \operatorname{Re} \sum_{n=0}^{m} n \mathrm{e}^{\mathrm{i}\alpha(m+\frac{1}{2}-n)} = \operatorname{Re} \mathrm{e}^{\alpha(m+\frac{1}{2})} \sum_{n=0}^{m} n \mathrm{e}^{-\mathrm{i}\alpha n} \\ &= \operatorname{Re} \mathrm{e}^{\alpha(m+\frac{1}{2})} \frac{n\mathrm{e}^{-\frac{3}{2}\mathrm{i}\alpha} - (n+1)\mathrm{e}^{-\frac{1}{2}\mathrm{i}\alpha} + \mathrm{e}^{-\mathrm{i}\alpha}}{(1-\mathrm{e}^{-\mathrm{i}\alpha})^2} \\ &= \frac{\cos \frac{1}{2}\alpha - \cos \alpha(m + \frac{1}{2})}{2(1-\cos\alpha)} = \frac{\sin \frac{1}{2}\alpha m \sin \frac{1}{2}\alpha(m+1)}{1 - \cos\alpha}.\end{aligned}$$

Proposition 2 *For every Riemann integrable odd function f it is true that*

$$\sigma_m[f](x) = \int_{-1}^{1} f(\xi) \tilde{F}_m(x-\xi) \mathrm{d}\xi, \tag{2.6}$$

where

$$\tilde{F}_m(x) = \frac{1}{m} \frac{\sin(\frac{1}{2}\pi m x) \sin[\frac{1}{2}\pi(m+1)x]}{1 - \cos \pi x}. \tag{2.7}$$

Proof It follows from our analysis, the oddity of f and the evenness of $\tilde{F}_m$ that

$$\begin{aligned}\sigma_m[f](x) &= \tfrac{1}{2} \int_{-1}^{1} f(\xi)[\tilde{F}_m(x-\xi) - \tilde{F}_m(x+\xi)] \mathrm{d}\xi \\ &= \tfrac{1}{2} \int_{-1}^{1} f(\xi) \tilde{F}_m(x-\xi) \mathrm{d}\xi - \tfrac{1}{2} \int_{-1}^{1} f(-\xi) \tilde{F}_m(x-\xi) \mathrm{d}\xi \\ &= \int_{-1}^{1} f(\xi) \tilde{F}_m(x-\xi) \mathrm{d}\xi\end{aligned}$$

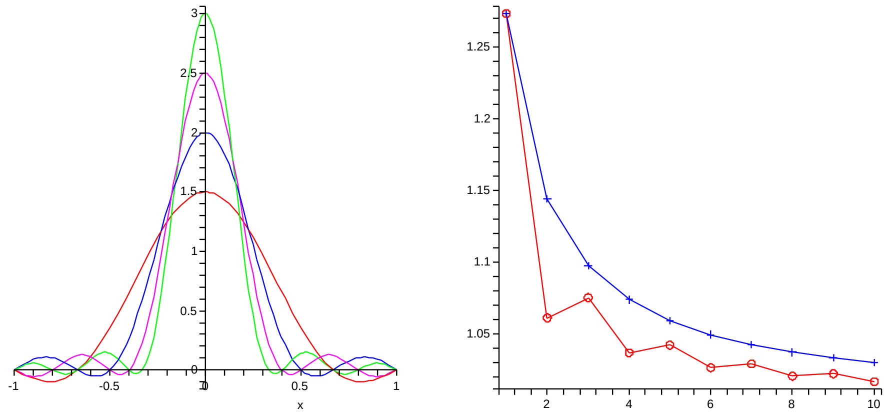

Figure 2.3: The kernels $\tilde{F}_m$ for $m = 2, 3, 4, 5$ on the left and the integrals $\int_{-1}^{1} \tilde{F}_m(x)\mathrm{d}x$ (circles) and $\int_{-1}^{1} |\tilde{F}_m(x)|\mathrm{d}x$ (pluses) on the right.

and (2.6) follows. □

The *kernel* $\tilde{F}_m$ bears resemblance to the classical Fejér kernel

$$F_m(x) = \frac{1}{m}\left[\frac{\sin\frac{1}{2}\pi(m+1)x}{\sin\frac{1}{2}\pi x}\right]^2$$

of Fourier analysis, with one important difference: While $F_m(x) \geq 0$ for $x \in [-1, 1]$ and $\int_{-1}^{1} F_m(x)\mathrm{d}x = 1$, neither statement is true for $\tilde{F}_m$. This is evident from Fig. 2.3 and will cause minor difficulties in our generalization of the Fejér theorem.

Proposition 3 *It is true that*

$$\int_{-1}^{1} \tilde{F}_m(x)\mathrm{d}x = 1 + \mathcal{O}\big(m^{-1}\big)\,, \qquad m \gg 1.$$

Proof We go back to an intermediate step in our derivation of $\tilde{F}_m$. Since f is odd,

$$\begin{aligned}\sigma_m[f](x) &= \frac{1}{2m}\int_{-1}^{1} f(\xi)\sum_{n=1}^{m}(m-n+1)[\cos\pi(n-\tfrac{1}{2})(x-\xi) - \cos\pi(n-\tfrac{1}{2})(x+\xi)]\mathrm{d}\xi \\ &= \frac{1}{m}\int_{-1}^{1} f(\xi)\sum_{n=1}^{m}(m-n+1)\cos\pi(n-\tfrac{1}{2})(x-\xi)\mathrm{d}\xi\end{aligned}$$

and we have

$$\int_{-1}^{1}\tilde{F}_m(x)\mathrm{d}x = \frac{1}{m}\int_{-1}^{1}\sum_{n=1}^{m}(m-n+1)\cos\pi(n-\tfrac{1}{2})x\mathrm{d}x = \frac{2}{m\pi}\sum_{n=1}^{m}(-1)^{n-1}\frac{m-n+1}{n-\frac{1}{2}}$$

$$= \frac{2}{m\pi}\left[-\sum_{n=0}^{m-1}(-1)^n + (m+\tfrac{1}{2})\sum_{n=0}^{m-1}\frac{(-1)^n}{n+\frac{1}{2}}\right]$$
$$= \frac{2}{m\pi}\left\{(2m+1)\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1} - (2m+1)\sum_{n=m}^{\infty}\frac{(-1)^n}{2n+1} - \tfrac{1}{2}[1-(-1)^m]\right\}.$$

Since $\sum_{n=0}^{\infty}(-1)^n/(2n+1) = \frac{1}{4}\pi$, we have

$$\int_{-1}^{1}\tilde{F}_m(x)\mathrm{d}x = 1 + \frac{1}{2m} - \frac{4m+2}{m\pi}\sum_{n=m}^{\infty}\frac{(-1)^n}{2n+1} - \frac{1-(-1)^m}{m\pi}.$$

The proposition follows, since convergent alternating series with monotone terms can be bounded in absolute value by the magnitude of its leading term. □

Proposition 4 *The bound*

$$\int_{-1}^{1}|\tilde{F}_m(x)|\mathrm{d}x \le \frac{4}{\pi} + \mathcal{O}\big(m^{-1}\big) \tag{2.8}$$

is valid for all $m \gg 1$.

Proof It follows from (2.7) that, given $\varepsilon \in (0,1)$,

$$\int_{-1}^{1}|\tilde{F}_m(x)|\mathrm{d}x = \frac{1}{m}\int_{-1}^{1}\frac{|\sin(\frac{1}{2}\pi m x)\sin(\frac{1}{2}(m+1)x)|}{1-\cos\pi x}\mathrm{d}x$$
$$= \frac{2}{m}\int_{0}^{\varepsilon}\frac{|\sin(\frac{1}{2}\pi m x)\sin(\frac{1}{2}(m+1)x)|}{1-\cos\pi x}\mathrm{d}x$$
$$+ \frac{2}{m}\int_{\varepsilon}^{1}\frac{|\sin(\frac{1}{2}\pi m x)\sin(\frac{1}{2}(m+1)x)|}{1-\cos\pi x}\mathrm{d}x = \frac{2}{m}(I_0+I_1).$$

Now, the inequality

$$I_1 \le \int_{\varepsilon}^{1}\frac{\mathrm{d}x}{1-\cos\pi x} = \frac{\cos(\frac{1}{2}\pi\varepsilon)}{\pi}$$

is obvious, since

$$-\frac{1}{\pi}\frac{\mathrm{d}\cot(\frac{1}{2}\pi x)}{\mathrm{d}x} = \frac{1}{1-\cos\pi x}.$$

Moreover, it is trivial to verify that

$$\frac{\sin(\frac{1}{2}\pi m\pi x)\sin[\frac{1}{2}\pi(m+1)x]}{1-\cos\pi x} = \tfrac{1}{2}\mathrm{U}_{m-1}(\cos\tfrac{1}{2}\pi x)\mathrm{U}_m(\cos\tfrac{1}{2}\pi x),$$

where U_n is the degree-n *Chebyshev polynomial of the second kind.* Since $|\mathrm{U}_n(x)| \le n+1$ for $x \in [-1,1]$ (Rainville 1960), we deduce that $I_0 \le \frac{1}{2}m(m+1)\varepsilon$. This results in the upper bound

$$\int_{-1}^{1}|\tilde{F}_m(x)|\mathrm{d}x \le \frac{2\cos(\frac{1}{2}\pi\varepsilon)}{m\pi} + (m+1)\varepsilon.$$

Given $m \geq 2$, we set $\varepsilon = \alpha/m$ for any $\alpha > 0$ and this results in

$$\int_{-1}^{1} |\tilde{F}_m(x)| \mathrm{d}x \leq \left(\alpha + \frac{4}{\pi^2 \alpha} \right) + \mathcal{O}\big(m^{-1}\big) .$$

The bound (2.8) follows by setting $\alpha = 2/\pi$. □

It is evident from Fig. 2.3 that the numbers $\kappa_m = \int_{-1}^{1} |\tilde{F}_m(x)| \mathrm{d}x$ form a strictly monotonically decreasing sequence. Direct computation shows that $\kappa_1 = 4/\pi$ and the figure seems to indicate that $\kappa_m \downarrow 1$. Proposition 4 is weaker than this statement, but perfectly adequate for our needs.

Theorem 5 *Let f be a Riemann integrable function in $[-1, 1]$. At every $x \in [-1, 1]$ where f is Lipschitz it is true that*

$$\lim_{m \to \infty} \sigma_m[f](x) = f(x).$$

In particular, modified Fourier series (1.3) is summable to f at every point of continuity.

Proof Essentially, we rehash the original Lipót Fejér's proof of the equivalent result for the classical Fourier series (1.1), except that we need to exercise much greater care. Since f is Riemann integrable, $M = \|f\|_\infty < \infty$. We commence by extending f outside $[-1, 1]$ by periodicity, whence

$$\sigma_m[f](x) = \int_{-1}^{1} f(\xi) \tilde{F}_m(x - \xi) \mathrm{d}\xi = \int_{x-1}^{x+1} f(x - \xi) \tilde{F}_m(\xi) \mathrm{d}\xi = \int_{-1}^{1} f(x - \xi) \tilde{F}_m(\xi) \mathrm{d}\xi.$$

Because f is Lipschitz at x, for every $\varepsilon > 0$ there exists $\delta = \delta(x, \varepsilon)$ such that

$$|f(x) - f(t)| \leq \frac{\pi \varepsilon}{4} \qquad \text{for every} \qquad |x - t| \leq \delta.$$

For every $|x| > \delta$ we have

$$|\tilde{F}_m(x)| \leq \frac{1}{m} \frac{1}{1 - \cos \pi \delta},$$

therefore there exists $m_0 \in \mathbb{N}$ such that

$$|\tilde{F}_m(x)| \leq \frac{\pi \varepsilon}{8M}, \qquad m \geq m_0, \quad |x| > \delta.$$

We now use Proposition 3 to argue that

$$\begin{aligned} |\sigma_m[f](x) - f(x)| &= \left| \int_{-1}^{1} f(x - \xi) \tilde{F}_m(\xi) \mathrm{d}\xi - f(x) \int_{-1}^{1} \tilde{F}_m(\xi) \mathrm{d}\xi \right| + \mathcal{O}\big(m^{-1}\big) \\ &= \left| \int_{-1}^{1} [f(x - \xi) - f(x)] \tilde{F}_m(\xi) \mathrm{d}\xi \right| + \mathcal{O}\big(m^{-1}\big) \\ &\leq \int_{|\xi| \leq \delta} |f(x - \xi) - f(x)| |\tilde{F}_m(\xi)| \mathrm{d}\xi \\ &\quad + \int_{\delta < |\xi| \leq 1} |f(x - \xi) - f(x)| |\tilde{F}_m(\xi)| \mathrm{d}\xi + \mathcal{O}\big(m^{-1}\big) \end{aligned}$$

$$\leq \frac{\pi\varepsilon}{4}\int_{|\xi|\leq\delta}|\tilde{F}_m(\xi)|\mathrm{d}\xi + \frac{\pi\varepsilon}{8M}(2M)\int_{\delta<|\xi|\leq 1}|\tilde{F}_m(\xi)|\mathrm{d}\xi + \mathcal{O}\big(m^{-1}\big)$$
$$\leq \frac{\pi\varepsilon}{4}\int_{-1}^{1}|\tilde{F}_m(\xi)|\mathrm{d}\xi + \mathcal{O}\big(m^{-1}\big)\,.$$

We conclude that $|\sigma_m[f](x)-f(x)|<\varepsilon$ by virtue of the inequality (2.8), thereby completing the proof. □

We progress next mirroring steps in the proof of the de la Vallée Poussin theorem (Körner 1988). For every $n=0,1,\ldots,m-1$ we set

$$\sigma_{n,m}[f](x) = \frac{1}{m-n}[(m+1)\sigma_m[f](x)-(n+1)\sigma_n[f](x)]$$

Theorem 6 *Suppose that f is Riemann integrable in $[-1,1]$ and that*

$$\hat{f}_n^C, \hat{f}_n^S = \mathcal{O}\big(n^{-1}\big)\,, \qquad n\gg 1. \tag{2.9}$$

If f is Lipschitz at $x\in(-1,1)$ then $S_m[f]\to f(x)$ as $m\to\infty$. Moreover, this progression to a limit is uniform in $[\alpha,\beta]$, where $-1<\alpha<\beta<1$, provided that $f\in \mathrm{C}[\alpha,\beta]$.

Proof As before, it is enough to prove the theorem for an odd function f.

Let f be Lipschitz at $x\in(-1,1)$. Then for every fixed $k\in\mathbb{Z}_+$

$$\sigma_{kn,(k+1)n}[f](x) = (k+1)\sigma_{(k+1)n}[f](x) - k\sigma_{kn}[f](x) + \frac{\sigma_{(k+1)n}[f](x)-\sigma_{kn}[f](x)}{n}.$$

Therefore, Theorem 5 implies that

$$\lim_{n\to\infty}\sigma_{kn,(k+1)n}[f](x) = f(x).$$

Moreover, if $f\in\mathrm{C}[\alpha,\beta]$ then, by an identical argument, $\sigma_{kn,(n+1)n}[f]$ converges uniformly to f for $[\alpha,\beta]$.

Finally, because of (2.9), there exist $\gamma>0$ and $j_0\in\mathbb{N}$ such that $|\hat{f}_j^S|\leq\gamma/j$ for $j\geq j_0$. Therefore, for any $n\geq 1$ and sufficiently large k, for every m such that $kn\leq m<(k+1)n$ and a point $x\in(-1,1)$ where f is Lipschitz, we have

$$|\sigma_{kn,(k+1)n}[f](x)-S_m[f](x)| \leq \sum_{j=kn+1}^{(k+1)n}|\hat{f}_j^S| \leq \frac{\gamma}{kn}n = \frac{\gamma}{k} \stackrel{k\to\infty}{\longrightarrow} 0.$$

The theorem follows. □

The de la Vallée Poussin-like Theorem 6 also provides an upper bound on the rate of convergence at Lipschitz points: Subject to (2.9), it is true that

$$S_m[f](x) = f(x) + \mathcal{O}\big(m^{-1}\big)\,, \qquad m\gg 1. \tag{2.10}$$

Note, however, that (at least in an asymptotic sense) a stronger condition holds for analytic functions. By virtue of (2.1) and (2.3), we have

$$\hat{f}_n^C, \hat{f}_n^S \sim \mathcal{O}\big(n^{-2}\big)\,, \qquad n\gg 1. \tag{2.11}$$

Can this be used to argue that in this particular case we can replace $\mathcal{O}\big(m^{-1}\big)$ by $\mathcal{O}\big(m^{-2}\big)$ in (2.10)? This certainly is a behaviour indicated by Fig. 2.1 and numerous other numerical experiments.

Had it been true that

$$\sigma_m[f](x) = f(x) + \mathcal{O}\big(m^{-2}\big)\,, \qquad m \gg 1, \tag{2.12}$$

for any analytic function f and $x \in (-1,1)$ (of course, we may no longer assume that f is odd), it would have been possible, at little additional effort, to strengthen the result of Theorem 6 and prove that convergence in (2.10) is indeed $\mathcal{O}\big(m^{-2}\big)$. Unfortunately, numerical experiments indicate that (2.12) is wrong. Therefore, although we do believe that the stronger result is true, it must remain a conjecture for the time being.

Of course, unless f is analytic, there is little hope for (2.11) to hold. For example, for the (odd) sign function

$$f(x) = \begin{cases} 1, & x \ge 0, \\ -1, & x < 0, \end{cases}$$

we have $\hat{f}_n^S = 2/[\pi(n-\frac{1}{2})]$ (and $\hat{f}_n^D = 2[1-(-1)^n]/(\pi n)$).

2.4 Convergence at the endpoints

Suppose that f is analytic in $[-1,1]$. In that case, by the de la Vallée Poussin theorem and its extension, Theorem 6, both classical and modified Fourier expansions converge pointwise and uniformly in any closed interval $[\alpha,\beta] \subset (-1,1)$. Although expansion coefficients decay faster for the modified expansion, as $\mathcal{O}\big(m^{-2}\big)$ compared with $\mathcal{O}\big(m^{-1}\big)$, and numerical results indicate the superiority of (1.3) over (1.1), the latter statement is currently not accompanied by a valid proof. However, another important advantage of the modified expansion is its behaviour at the endpoints ± 1.

Unless f is periodic, its classical Fourier expansion at the endpoints fails to converge to the exact value of f: it is true that

$$\lim_{x\to\pm 1} \mathcal{F}_m[f](x) = \tfrac{1}{2}[f(-1)+f(1)]. \tag{2.13}$$

Recall our partition $f = f_e + f_o$ into even and odd functions. It is clear from (2.13) that the Fourier expansion of f_e converges to the right value $f_e(-1) = f_e(1)$ at the endpoints. Since $\mathcal{M}_m[f_e] = \mathcal{F}_m[f_e]$, this is also the case for modified Fourier. Therefore, again, we are allowed to restrict our gaze to odd functions f.

In our quest to examine the convergence of $\mathcal{M}_m[f]$ at the endpoints, we progress in two stages. Firstly, we examine in detail the function $f(x) = x^{2p+1}$, $p \in \mathbb{Z}_+$, denoting its Fourier-sine coefficients by $\varphi_{p,n} = \hat{f}_n^S$. Clearly, by straightforward calculation

$$\varphi_{0,n} = \frac{2(-1)^{n-1}}{[\pi(n-\frac{1}{2})]^2}, \qquad n \in \mathbb{N},$$

and, integrating twice by parts,

$$\varphi_{p,n} = (-1)^{n-1}\frac{2(2p+1)}{[\pi(n-\frac{1}{2})]^2} = \frac{(2p)(2p+1)}{[\pi(n-\frac{1}{2})]^2}\varphi_{p-1,n}, \qquad p,n \in \mathbb{N}.$$

Therefore, by induction,

$$\varphi_{p,n} = 2(-1)^{n-1} \sum_{k=0}^{p} (-1)^k \frac{(2p+1)!}{(2p-2k)!} \frac{1}{[\pi(n-\frac{1}{2})]^{2k+2}}, \qquad n \in \mathbb{N}. \tag{2.14}$$

Since $\sin \pi(n-\frac{1}{2}) = (-1)^{n-1}$, letting

$$S[f](x) = \lim_{m\to\infty} S_m[f](x), \qquad x \in [-1,1],$$

it follows from (2.14) that

$$S[f](1) = (-1)^{n-1} \sum_{n=1}^{\infty} \varphi_{p,n} = 2 \sum_{k=0}^{p} (-1)^k \frac{(2p+1)!}{(2p-2k)!} \sum_{n=0}^{\infty} \frac{1}{[\pi(n-\frac{1}{2})]^{2k+2}}.$$

According to (Abramowitz & Stegun 1964, p. 807),

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)^q} = \left(1 - \frac{1}{2^q}\right) \zeta(q), \qquad q \geq 2,$$

where ζ is the *Riemann zeta function.* Since $\zeta(2k+2) = (2\pi)^{2k+2} |\mathrm{B}_{2k+2}|/[2(2k+2)!]$, where B_j is the jth *Bernoulli number* (Abramowitz & Stegun 1964, p. 807), we deduce that

$$\sum_{n=0}^{\infty} \frac{1}{[\pi(n+\frac{1}{2})]^{2k+2}} = \tfrac{1}{2} 4^{k+1}(4^{k+1}-1) \frac{|\mathrm{B}_{2k+2}|}{(2k+2)!},$$

consequently

$$S[f](1) = \sum_{k=0}^{p} (-1)^k \frac{(2p+1)!}{(2p-2k)!} 4^{k+1}(4^{k+1}-1) \frac{|\mathrm{B}_{2k+2}|}{(2k+2)!}, \qquad p \in \mathbb{Z}_+. \tag{2.15}$$

Proposition 7 *It is true that* $S[f](1) = 1 = f(1)$.

Proof Letting $|\mathrm{B}_{2k+2}| = (-1)^{k+1}\mathrm{B}_{2k+2}$, $k \in \mathbb{Z}_+$ in (2.15), we need to prove the identity

$$\sum_{k=0}^{p} \frac{(2p+1)!}{(2p-2k)!(2k+2)!} \mathrm{B}_{2k+2} 4^{k+1}(4^{k+1}-1) = 1.$$

This is equivalent to

$$\sum_{k=0}^{p} \frac{\mathrm{B}_{2k+2}}{(2k+2)!(2p-2k)!} 16^{k+1} - \sum_{k=0}^{p} \frac{\mathrm{B}_{2k+2}}{(2k+2)!(2p-2k)!} 4^{k+1} = \frac{1}{(2p+1)!}.$$

We shift the indices k by one and add an equal term to each sum: the outcome is another identity equivalent to the statement of the proposition,

$$\sum_{k=0}^{q} \binom{2q}{2k} \mathrm{B}_{2k} 16^k - \sum_{k=0}^{q} \binom{2q}{2k} \mathrm{B}_{2k} 4^k = 2q,$$

where $q = p + 1 \in \mathbb{N}$. Recall however that $\mathrm{B}_{2k+1} = 0$, $k \in \mathbb{Z}_+$, except that $\mathrm{B}_1 = -\frac{1}{2}$. Therefore

$$\sum_{k=0}^{q} \binom{2q}{2k} \mathrm{B}_{2k} y^{2k} = \sum_{k=0}^{2q} \binom{2q}{k} \mathrm{B}_k y^k + qy, \qquad q \in \mathbb{N},$$

and it is enough to prove that

$$\sum_{k=0}^{2q} \binom{2q}{k} \mathrm{B}_k 4^k = \sum_{k=0}^{2q} \binom{2q}{k} \mathrm{B}_k 2^k. \tag{2.16}$$

Let $\mathrm{B}_k(\,\cdot\,)$ be the kth *Bernoulli polynomial* (Abramowitz & Stegun 1964, p.804) and recall that $\mathrm{B}_k = \mathrm{B}_k(0)$. Since

$$\mathrm{B}_n(x+h) = \sum_{k=0}^{n} \binom{n}{k} \mathrm{B}_k(x) h^{n-k}, \qquad n \in \mathbb{Z}_+, \quad x, h \in \mathbb{C},$$

(2.16) is equivalent to $\mathrm{B}_{2q}(\frac{1}{2}) = 4^q \mathrm{B}_{2q}(\frac{1}{4})$. This follows immediately from the duplication formula

$$\mathrm{B}_n(mx) = m^{n-1} \sum_{k=0}^{m-1} \mathrm{B}_n(x + \tfrac{k}{m})$$

and the identity $\mathrm{B}_n(1-x) = (-1)^n \mathrm{B}_n(x)$ (Abramowitz & Stegun 1964, p.804), letting $n = 2q$, $m = 2$ and $x = \frac{1}{4}$. Therefore the proposition is true. $\square$

Thus, $S_m[f](1) \to f(1)$ for $f(x) = x^{2p+1}$ and an identical argument proves convergence at the other endpoint. But what is the speed of convergence?

We revisit our analysis, replacing $S[f]$ with $S_m[f]$. Straightforward algebra confirms that

$$S_m[f](1) = S[f](1) - 2 \sum_{k=0}^{p} (-1)^k \frac{(2p+1)!}{(2p-2k)!} \sum_{n=m}^{\infty} \frac{1}{[\pi(n+\frac{1}{2})]^{2k+2}}. \tag{2.17}$$

However, it is easy to deduce from (Abramowitz & Stegun 1964, p.258) (or just trust `Maple`) that

$$\sum_{k=m}^{\infty} \frac{1}{(n+\frac{1}{2})^{2k+2}} = \frac{\mathrm{d}^{2k+1}\psi(m+\frac{1}{2})}{\mathrm{d}x^{2k+1}},$$

where ψ is the *digamma function.* Since

$$\psi(z) \sim \log z - \frac{1}{2z} - \sum_{r=0}^{\infty} \frac{\mathrm{B}_{2r}}{2r} \frac{1}{z^{2r}}, \qquad |z| \to \infty, |\arg z| < \pi$$

(Abramowitz & Stegun 1964, p.258), differentiation yields

$$\psi^{(2k+1)}(z) \sim \frac{(2k)!}{z^{2k+1}} + \frac{1}{2} \frac{(2k+1)!}{z^{2k+2}} - \sum_{r=1}^{\infty} \frac{(2r+2)!}{(2r)!} \frac{\mathrm{B}_{2r}}{z^{2r+2k+1}}, \qquad |z| \to \infty, |\arg z| < \pi.$$

Substitution in (2.17) results in the asymptotic expansion

$$S_m[f](1) - S[f](1) \sim -2\sum_{k=0}^{p} \frac{(2p+1)!}{(2p-2k)!}\frac{(-1)^k}{\pi^{2k+2}}\left[\frac{(2k)!}{(n+\frac{1}{2})^{2k+1}} + \frac{1}{2}\frac{(2k+1)!}{(n+\frac{1}{2})^{2k+2}} - \sum_{r=1}^{\infty}\frac{(2r+2k)!}{(2r)!}\frac{\mathrm{B}_{2r}}{(n+\frac{1}{2})^{2r+2k+1}}\right]. \tag{2.18}$$

We thus conclude that for $f(x) = x^{2p+1}$ it is true that

$$S_m[f](\pm 1) \sim S[f](\pm 1) + \mathcal{O}\big(m^{-1}\big)\,, \qquad m \gg 1.$$

Theorem 8 *Given an odd analytic function f, uniformly convergent in $[-1,1]$, it is true that*

$$S_m[f](\pm 1) \sim f(\pm 1) - \frac{2f'(\pm 1)}{\pi^2}\frac{1}{m+\frac{1}{2}} - \frac{f'(\pm 1)}{\pi^2}\frac{1}{(m+\frac{1}{2})^2} + \left[\frac{f'(\pm 1)}{3\pi^2} + \frac{4f'''(\pm 1)}{\pi^4}\right]\frac{1}{(m+\frac{1}{2})^3} + \mathcal{O}\big(m^{-4}\big)\,, \qquad m \gg 1.$$

Proof Given $f(x) = \sum_{p=0}^{\infty} f_p x^{2p+1}$, we multiply (2.18) by f_{2p+1} and sum up for $p \in \mathbb{Z}_+$. This results in the desired asymptotic expansion at $+1$, subject to easy algebraic manipulation. The expansion at $x = -1$ follows by symmetry. □

Given that $S_m[f](\pm 1) \sim f(\pm 1) + \mathcal{O}\big(m^{-1}\big)$ for any even f analytic in $[-1,1]$, we deduce that modified Fourier expansions for all analytic functions converge at the endpoints, albeit at the slower rate of $\mathcal{O}\big(m^{-1}\big)$.

3 Computing modified Fourier coefficients

3.1 The asymptotic method

The point of departure for the computation of $\hat{f}_n^C$ and $\hat{f}_n^S$ for $n \geq 1$ are the asymptotic expansions (2.1) and (2.3). Thus, given $s \in \mathbb{N}$, we let

$$\hat{A}_{s,n}^C[f] = (-1)^n \sum_{k=0}^{s-1} \frac{(-1)^k}{(n\pi)^{2k+2}}[f^{(2k+1)}(1) - f^{(2k+1)}(-1)], \tag{3.1}$$

$$\hat{A}_{s,n}^S[f] = (-1)^{n-1} \sum_{k=0}^{s-1} \frac{(-1)^k}{[(n-\frac{1}{2})\pi]^{2k+2}}[f^{(2k+1)}(1) + f^{(2k+1)}(-1)].$$

It follows at once that

$$\hat{A}_{s,n}^C[f] \sim \hat{f}_n^C + \mathcal{O}\big(n^{-2s-2}\big)\,, \qquad \hat{A}_{s,n}^S \sim \hat{f}_n^S + \mathcal{O}\big(n^{-2s-2}\big)\,, \qquad n \gg 1. \tag{3.2}$$

In Fig. 3.1 we display scaled errors for $s = 1, 2, 3$ for $f(x) = \mathrm{e}^x$ (numerous experiments with other choices of f result in qualitatively identical behaviour). Progression to a limit is

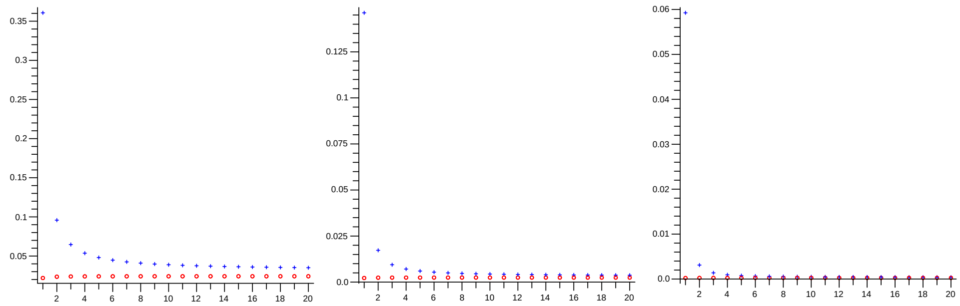

Figure 3.1: Scaled errors $n^{2s+2}|\hat{A}^C_{s,n}[f] - \hat{f}^C_n|$ (circles) and $n^{2s+2}|\hat{A}^S_{s,n}[f] - \hat{f}^S_n|$ (crosses) for $s = 1, 2, 3$ and $f(x) = \mathrm{e}^x$.

	Cosine terms				Sine terms		
n	$s=1$	$s=2$	$s=3$	n	$s=1$	$s=2$	$s=3$
1	-2.19_{-02}	2.22_{-03}	-2.25_{-04}	1	3.61_{-01}	-1.46_{-01}	5.93_{-02}
2	-1.47_{-03}	-3.73_{-05}	9.44_{-07}	2	-5.99_{-03}	2.70_{-04}	-1.21_{-05}
3	-2.95_{-04}	3.31_{-06}	-3.73_{-08}	3	-7.98_{-04}	-1.29_{-05}	2.10_{-07}
10	2.41_{-06}	-2.44_{-09}	2.47_{-12}	10	-3.89_{-06}	4.36_{-09}	-4.90_{-12}

Table 1: Absolute errors $\hat{A}^C_{s,n}[f] - \hat{f}^C_n$ (on the left) and $\hat{A}^S_{s,n}[f] - \hat{f}^S_n$ for $f(x) = \mathrm{e}^x$.

consistent with our asymptotic estimate but a significantly more valuable observation is that it occurs fairly rapidly. In other words, for every $s \in \mathbb{N}$, analytic f and given tolerance ε, there exists a fairly modest n_ε such that $|\hat{A}^C_{s,n}[f] - \hat{f}^C_n|, |\hat{A}^S_{s,n}[f] - \hat{f}^S_n| \le \varepsilon$ for all $n \ge n_\varepsilon$.

In Table 1 we display absolute errors for the first few coefficients for $f(x) = \mathrm{e}^x$. Clearly, the error is unacceptably large before the onset of asymptotic behaviour: *we are justified in using (3.1) only for sufficiently large* n. In other words, we compute the coefficients for small values of n by, say, Gaussian quadrature. However, once we implement (3.1) for $n \ge n_0$ for a suitable $n_0 \in \mathbb{N}$, we can obtain very precise approximation of the first m coefficients in $\mathcal{O}(m)$ operations, having we first computed $f^{(2k+1)}(\pm 1)$ for $k = 0, \ldots, s-1$. Subsequently, for each $n \ge n_0$ we form the two linear length-s combinations (3.1).

Overall, the asymptotic method (3.1) is promising, yet the error is unacceptably large for realistic values of s and moderate values of n. It is, however, just the first step on our quest to approximate modified Fourier coefficients by techniques from highly oscillatory quadrature.

3.2 Filon-type methods

The quadrature of highly oscillatory integrals of the form $I[f; g] = \int_a^b f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x$, where g is a real function and $\omega \gg 1$, has received much attention in the last few years (Huybrechs & Vandewalle 2006, Iserles & Nørsett 2005, Olver 2006). Many of these methods commence from an asymptotic expansion, similar in spirit to (3.1), as a point of departure to two more precise algorithms: Filon-type (Iserles & Nørsett 2005) and Levin-type methods (Olver 2006). In the present setting g is linear, thus Filon-type and Levin-type methods are identical. For reasons of presentation, we adopt the terminology of Filon-type methods.

Trivially, we can represent both $\hat{f}_n^C$ and $\hat{f}_n^S$ using integrals of the form $I[f;g]$:

$$\hat{f}_n^C = \tfrac{1}{2}\{I[f,x] + I[f,-x]\}, \qquad \hat{f}_n^S = \tfrac{1}{2\mathrm{i}}\{I[f\mathrm{e}^{-\frac{1}{2}\mathrm{i}x},x] - I[f\mathrm{e}^{\frac{1}{2}\mathrm{i}x},-x]\},$$

with $\omega = n$.

Let $-1 = c_1 < c_2 < \cdots < c_\nu = 1$ be ν given *quadrature nodes* and suppose that each c_k has *multiplicity* $m_k \in \mathbb{N}$. We form a polynomial p of degree $\sum_{k=1}^{\nu} m_k - 1$ such that

$$p^{(i)}(c_k) = f^{(i)}(c_k), \qquad k = 0,1,\ldots,m_k-1, \quad k = 1,2,\ldots,\nu,$$

and consider the quadrature formula

$$Q[f;g] = \int_a^b p(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x. \tag{3.3}$$

(We assume that $Q[f]$ can be evaluated explicitly: this is certainly true in the case $g(x) = \pm x$, which is of our concern in this paper.) In that case it has been proved in (Iserles & Nørsett 2005) that $Q[f;g] \sim I[f;g] + \mathcal{O}\big(\omega^{-s-1}\big)$, where $s = \min\{m_1, m_\nu\}$.

Since we seek to optimize the Filon-type method for the current setting, we recall from (Iserles & Nørsett 2005) that the above asymptotic estimate is proved by replacing f with $p-f$ in the asymptotic expansion of $I[f;g]$ in negative powers of ω. However, our expansions (2.1) and (2.3) employ only odd derivatives of f. In other words, once $p^{(2i+1)}(\pm 1) = f^{(2i+1)}(\pm 1)$ for $i = 0,1,\ldots,r-1$, say, then replacing f with $p-f$ in (2.1) and (2.3) proves at once that the asymptotic error of the relevant Filon-type method is $\mathcal{O}\big(n^{-2r-2}\big)$. In other words, *we need to interpolate only to odd derivatives!*

We can go a step further: Suppose that φ is a polynomial such that

$$\varphi^{(2i)}(c_k) = f^{(2i+1)}(c_k), \qquad i = 0,1,\ldots,m_k-1, \quad k = 1,2,\ldots,\nu, \tag{3.4}$$

and set $p(x) = f(0) + \int_0^x \varphi(\xi)\mathrm{d}\xi$. Then $p^{(2i+1)}$ matches $f^{(2i+1)}$ at the nodes (and at no extra price $p(0) = f(0)$) and the asymptotic error of the Filon-type method

$$\tilde{F}_{s,n}^C[f] = \int_{-1}^1 p(x)\cos\pi n x\mathrm{d}x, \qquad \tilde{F}_{s,n}^S[f] = \int_{-1}^1 p(x)\sin\pi(n-\tfrac{1}{2})x\mathrm{d}x \tag{3.5}$$

is $\mathcal{O}\big(n^{-2s-2}\big)$. Here $s = \min\{m_1, m_\nu\}$.

It is trivial to observe that $\nu = 2$ and $m_1 = m_2 = s$ results in the asymptotic method (3.1) and nothing is gained. The advantage of (3.5), though, is that we can use intermediate points $c_k \in (-1,1)$ to boost precision. Firstly, however, we express (for $n \geq 1$) the integrals in (3.5) in terms of the polynomial φ. Specifically, integrating by parts,

$$\hat{F}_{s,n}^C[f] = -\frac{1}{n\pi}\int_{-1}^1 \varphi(x)\sin\pi n x\mathrm{d}x, \qquad \hat{F}_{s,n}^S[f] = \frac{1}{(n-\frac{1}{2})\pi}\int_{-1}^1 \varphi(x)\cos\pi(n-\tfrac{1}{2})x\mathrm{d}x. \tag{3.6}$$

The method (3.6) cannot be used for approximating $\hat{f}_0^C$ and is less precise for small values of n, before the onset of asymptotic behaviour. Our proposal is to reuse for such values of n the data in (3.4), together with the value $f(0)$, in a classical quadrature scheme

$$\hat{Q}_s[h] = 2h(0) + \sum_{k=1}^{\nu} \sum_{i=0}^{m_k-1} b_{k,i} h^{(2i+1)}(c_k) \approx \int_{-1}^{1} h(x)\mathrm{d}x. \tag{3.7}$$

We let $h(x) = f(x)$ for the computation of $\hat{f}_0^C$ and $h(x) = f(x)\cos\pi n x$ or $h(x) = f(x)\sin\pi(n-\frac{1}{2})x$ for the approximation of $\hat{f}_n^C$ or $\hat{f}_n^S$, respectively, for small values of n. The weights $b_{k,i}$ are chosen to maximise the (classical) order of (3.7), i.e. render it exact for polynomials of the highest-possible degree.

Other things being equal, we found it a good strategy to choose the intermediate points $c_2,\ldots,c_{\nu-1}$ to maximise the order of (3.7). It is reasonable to choose symmetric setting, $c_{\nu+1-k} = -c_k$ and $m_{\nu+1-k} = m_k$, whereby it follows at once from symmetry considerations that $b_{\nu+1-k,i} = -b_{k,i}$.

The simplest example with $\nu \ge 3$ is $\boldsymbol{c} = [-1, 0, 1]$ and $\boldsymbol{m} = [1, 1, 1]$. Therefore,

$$\varphi(x) = f'(0) + \tfrac{1}{2}[f'(1) - f'(-1)]x + \tfrac{1}{2}[f'(1) - 2f'(0) + f'(-1)]x^2$$

and

$$\begin{aligned} \hat{F}_{1,n}^C[f] &= \hat{A}_{1,n}^C[f], \\ \hat{F}_{1,n}^S[f] &= \hat{A}_{1,n}^S[f] - \frac{2(-1)^{n-1}}{[(n-\frac{1}{2})\pi]^4}[f'(1) - 2f'(0) + f'(-1)]. \end{aligned}$$

The underlying quadrature (3.7) is

$$\hat{Q}_1[h] = 2h(0) + \tfrac{1}{6}[h'(1) - h'(-1)]$$

and it is of order 4.

Although numerical experiments indicate that $\hat{F}_{1,n}^S$ produces much smaller error that $\hat{A}_{1,n}^S$, we do not pursue this particular choice since $\hat{F}_{1,n}^C = \hat{A}_{1,n}^C$. Instead, consider the *Gauss–Lobatto nodes*

$$\boldsymbol{c} = [\ -1 \quad -\tfrac{\sqrt{11}}{7} \quad \tfrac{\sqrt{11}}{7} \quad 1\ ], \qquad \boldsymbol{m} = [\ 1 \quad 1 \quad 1 \quad 1\ ].$$

This choice yields

$$\begin{aligned} \hat{F}_{1,n}^C[f] &= \hat{A}_{1,n}^C[f] - \tfrac{147}{209}\frac{(-1)^n}{(n\pi)^4}\{11[f'(1) - f'(-1)] - 7\sqrt{11}[f'(\tfrac{\sqrt{11}}{7}) - f'(-\tfrac{\sqrt{11}}{7})]\}, \\ \hat{F}_{1,n}^S[f] &= \hat{A}_{1,n}^S[f] - \tfrac{49}{19}\frac{(-1)^{n-1}}{[(n-\frac{1}{2})\pi]^4}[f'(1) - f'(\tfrac{\sqrt{11}}{7}) - f'(-\tfrac{\sqrt{11}}{7}) + f'(-1)]. \end{aligned} \tag{3.8}$$

The reason for this particular choice of nodes is to maximise the order of (3.7):

$$\hat{Q}_2[h] = 2h(0) + \tfrac{37}{2280}[h'(1) - h'(-1)] + \tfrac{2401\sqrt{11}}{25080}[h'(\tfrac{\sqrt{11}}{7}) - h'(-\tfrac{\sqrt{11}}{7})],$$

of order 8.

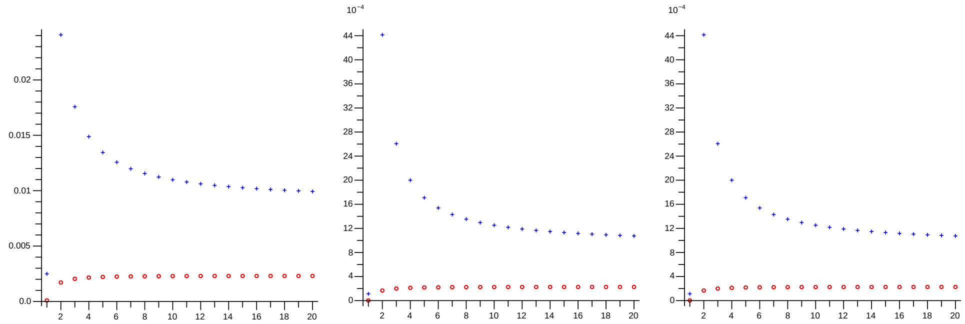

Figure 3.2: Scaled errors $n^{2s+2}|\hat{F}^C_{s,n}[f]-\hat{f}^C_n|$ (circles) and $n^{2s+2}|\hat{F}^S_{s,n}[f]-\hat{f}^S_n|$ (crosses) for (a) $s=1$, $\boldsymbol{c}=[-1.-\frac{\sqrt{11}}{7},\frac{\sqrt{11}}{7},1]$, $\boldsymbol{m}=[1,1,1,1]$; (b) $s=2$, $\boldsymbol{c}=[-1,-a,a,1]$, $a=\frac{1}{1860}\sqrt{2937870-930\sqrt{5879841}}$, $\boldsymbol{m}=[2,1,1,2]$; and (c) $s=2$, $\boldsymbol{c}=[-1,-a,a,1]$, $a\approx .74158177109$, $\boldsymbol{m}=[2,2,2,2]$; with $f(x)=\mathrm{e}^x$.

The errors produced by the method (3.8) for $f(x)=\mathrm{e}^x$ have been displayed in Fig. 3.2 (on the left) and in the first column of Table 2. Comparison with relevant data for the asymptotic method (with $s=1$) in Fig. 3.1 and Table 1 confirms that, while asymptotic error is $\mathcal{O}(n^{-4})$ and difference is small for $n\gg 1$, for moderate values of n we attain much higher accuracy with (3.8).

Our first example of a Filon method for $s=2$ is

$$\boldsymbol{c}=[\begin{array}{cccc}-1 & -\alpha & \alpha & 1\end{array}],\quad \text{where}\quad \alpha=\frac{1}{1860}\sqrt{2937870-930\sqrt{5879841}}$$

and $\boldsymbol{m}=[2,1,1,2]$. The reason for this choice is that the quadrature formula (3.7) is of order 10, and this is the best we can attain with this configuration of data. The corresponding Filon-type method is presented underneath: note that in practical applications one is likely to use floating point numbers.

$$\begin{aligned}
\hat{F}^C_{2,n}[f] &= \hat{A}^C_{2,n}[f]+\frac{(-1)^n}{(n\pi)^6}\left\{\frac{40397049-27369\sqrt{5879841}}{371008}[f'(1)-f'(-1)]\right.\\
&\quad+\frac{16655545269+23030811\sqrt{5879841}}{204425408}\alpha[f'(\alpha)-f'(-\alpha)] \qquad (3.9)\\
&\quad\left.+\frac{16563-3\sqrt{5879841}}{992}[f'''(1)-f'''(-1)]\right\}\\
\hat{F}^S_{2,n}[f] &= \hat{A}^S_{2,n}[f]+\frac{(-1)^{n-1}}{[(n-\frac12)\pi]^6}\left\{\frac{2183363-24003\sqrt{5879841}}{5844872}[f'(1)-f'(\alpha)\right.\\
&\quad\left.-f'(-\alpha)+f(1)]+\frac{46323-3\sqrt{5879841}}{15628}[f'''(1)+f'''(-1)]\right\}.
\end{aligned}$$

Cosine terms

n	$\boldsymbol{m}=[1,1,1,1]$	$\boldsymbol{m}=[2,1,1,2]$	$\boldsymbol{m}=[2,2,2,2]$
0	1.65_{-06}	-1.98_{-08}	3.90_{-10}
1	-8.87_{-05}	2.38_{-06}	-4.08_{-09}
2	1.07_{-04}	-2.62_{-06}	9.84_{-10}
3	2.52_{-05}	2.76_{-07}	3.62_{-09}
10	2.28_{-07}	-2.26_{-10}	-5.19_{-12}

Sine terms

n	$\boldsymbol{m}=[1,1,1,1]$	$\boldsymbol{m}=[2,1,1,2]$	$\boldsymbol{m}=[2,2,2,2]$
1	-2.49_{-03}	1.13_{-04}	-1.35_{-06}
2	1.50_{-03}	6.90_{-05}	-3.21_{-07}
3	2.17_{-04}	-3.58_{-06}	-8.26_{-08}
10	-1.10_{-06}	1.25_{-09}	4.71_{-11}

Table 2: Absolute errors $\hat{F}^C_{s,n}[f]-\hat{f}^C_n$ (top) and $\hat{F}^S_{s,n}[f]-\hat{f}^S_n$ for $f(x)=\mathrm{e}^x$. The errors for $\hat{f}^C_0$ were produced with $\hat{Q}_s[f]$. Note that $s=1$ for the rightmost column, otherwise $s=2$.

The middle plot in Fig. 3.2 and the middle column of Table 2 demonstrate that (3.9) behaves as predicted by theory. Comparison with the middle column of Table 1 confirms that a remarkable improvement in accuracy can be attained at a price of a single extra derivative evaluation.

An alternative to (3.9) is to consider

$$\boldsymbol{c}=[\ -1\quad -\beta\quad \beta\quad 1\ ],\qquad \boldsymbol{m}=[\ 2\quad 2\quad 2\quad 2\ ],$$

where we choose $\beta\approx 0.74158177109350494340800 0$ as a zero of the polynomial $51150x^8-136939x^6+88847x^4-18373x^2+1331$: this ensures that (3.7) is of order 12. We do not bother to derive $\hat{F}^C_{2,n}$ and $\hat{F}^S_{2,n}$ in an explicit form. Although this can be done in a straightforward computation, little additional insight will be gained. The rightmost plot in Figure 3.2 demonstrates conformity with $\mathcal{O}\big(n^{-6}\big)$ decay of the error. More notably, the right column of Table 2 underscores truly striking performance of the method for *all* n, inclusive of $n=0$. The reason is as follows: while for large ns precision is assured by rapid decay of asymptotic expansion, for small n it is caused by the high order of the underlying classical quadrature.

3.3 Design and implementation of Filon-type methods

All three Filon-type methods of the last subsection share a common structural feature. We are given distinct nodes $\boldsymbol{c}\in[-1,1]^\nu$ with $c_1=-1$, $c_\nu=1$ and multiplicities $\boldsymbol{m}\in\mathbb{N}^\nu$, where $s=\min\{m_1,m_\nu\}$. In other words, our methods use the data

$$f(0),\qquad f^{(2i+1)}(c_k),\quad i=0,1,\ldots,m_k-1,\quad k=1,2,\ldots,\nu. \tag{3.10}$$

The Filon-type method can be written in the form

$$\hat{F}^C_{s,n}[f]=\hat{A}^C_{s,n}[f]+\frac{(-1)^n}{(n\pi)^{2s+2}}\hat{\mathcal{E}}^C_{s,n}[f], \tag{3.11}$$

$$\hat{F}^S_{s,n}[f] = \hat{A}^S_{s,n}[f] + \frac{(-1)^{n-1}}{[(n-\frac{1}{2})\pi]^{2s+2}}\hat{\mathcal{E}}^S_{s,n}[f],$$

where

$$\hat{\mathcal{E}}^C_{s,n}[f] = \sum_{k=1}^{\nu}\sum_{i=0}^{m_k-1}\theta^C_{k,i}f^{(2i+1)}(c_k),$$
$$\hat{\mathcal{E}}^S_{s,n}[f] = \sum_{k=1}^{\nu}\sum_{i=0}^{m_k-1}\theta^S_{k,i}f^{(2i+1)}(c_k).$$

Note that the coefficients $\theta^C_{k,i}$ and $\theta^C_{k,i}$ are *independent of* n. This immediately provides us with an efficient algorithm for the computation of the first m modified Fourier coefficients:

1. Compute derivatives (3.10);
2. Form the linear combinations $(-1)^k[f^{(2k+1)}(1) \mp f^{(2k+1)}(1)]$, $k = 0,1,\ldots,s-1$, $\hat{\mathcal{E}}^C_{s,n}[f]$ and $\hat{\mathcal{E}}^S_{s,n}[f]$;
3. Approximate $\hat{f}^C_0$ and $\hat{f}^S_1$ with the underlying classical quadrature (3.7);
4. Evaluate (3.11) for all remaining coefficients by forming for each $\hat{f}^C_n$ and $\hat{f}^S_n$ a linear combination of $s+1$ terms.

The above algorithm requires $\mathcal{O}(m)$ flops (recall that FFT 'costs' $\mathcal{O}(m\log_2 m)$ flops). Moreover, unlike FFT, it is *fully adaptive:* we can go on evaluating modified Fourier coefficients for as long as we wish or until we decide that they have become sufficiently small and the computation may terminate. There is absolutely no need to fix the number of coefficients in advance!

The *raison d'etre* of (3.11) being an asymptotic expansion, we are justified in using it only for sufficiently large n, although numerical experiments demonstrate that for $s \geq 2$ and $\nu \geq 4$ "sufficiently large n" means in this context $n \geq 1$. Yet, for $n = 0$ (and perhaps for few other small values of n) we use the underlying classical quadrature (3.7) with $h(x) = f(x)$ or (for $n \geq 1$) $h(x) = f(x)\cos\pi nx$ and $h(x) = f(x)\sin\pi(n-\frac{1}{2})x$. Given multiplicities $\boldsymbol{m}$, we choose internal nodes $c_2,\ldots,c_{\nu-1}$ to maximise the (classical) order of (3.7). Note that general theory for this quadrature is missing and in the last subsection we have resorted to *ad hoc* order analysis.

Numerical experiments indicate that even for small values of $n \geq 1$ (3.11) is almost always superior to (3.7). Thus (compare with the rightmost column of Table 2) using (3.7) to compute modified Fourier coefficients with the third (hence, most precise) method of last subsection results in the following errors:

n	cosine	sine
1	-4.64_{-04}	-2.73_{-07}
2	1.37_{-02}	-2.68_{-02}

The reason is that the error of the 12-order quadrature (3.7) scales like the twelfth derivative of the underlying function, and the latter grows rapidly for all coefficients except for $\hat{f}^C_0$ and $\hat{f}^S_1$.

Intriguingly, Filon-type methods (3.11) lend themselves to an alternative interpretation. Comparing (3.11) with (3.1), we observe that

$$\hat{F}^C_{s,n}[f] - \hat{A}^C_{s+1,n}[f] = \frac{(-1)^n}{(n\pi)^{2s+2}}\{\hat{\mathcal{E}}^C_{s,n}[f] - (-1)^{s+1}[f^{(2s+1)}(1) - f^{(2s+1)}(-1)]\},$$
$$\hat{F}^S_{s,n}[f] - \hat{A}^S_{s+1,n}[f] = \frac{(-1)^n}{[(n-\frac{1}{2})\pi]^{2s+2}}\{\hat{\mathcal{E}}^S_{s,n}[f] - (-1)^{s+1}[f^{(2s+1)}(1) + f^{(2s+1)}(-1)]\}.$$

This implies a design principle for (3.11) which is completely different to the rationale underlying Filon-type methods: we choose the coefficients $\theta^C_{k,i}$ and $\theta^S_{k,i}$ to ensure that

$$\hat{\mathcal{E}}^C_{s,n}[h] = (-1)^{s+1}[h^{(2s+1)}(1) - h^{(2s+1)}(-1)],$$
$$\hat{\mathcal{E}}^S_{s,n}[h] = (-1)^{s+1}[h^{(2s+1)}(1) + h^{(2s+1)}(-1)]$$

for $h \in \mathbb{P}_r$ (the set of polynomials of degree $\leq r$) for the largest possible value of $r \in \mathbb{Z}_+$. Ideally, we might hope for $r = \sum_{k=1}^{\nu} m_k - 1$, but this simplistic argument, based on counting the number of degrees of freedom in (3.10), might well be naive. This issue, as well as the design of the underlying classical quadrature (3.7), are a matter for future research.

This is perhaps the place to emphasize that a Filon-type method with s is not simply an approximation to the asymptotic method with $s+1$: as can be confirmed from Tables 1 and 2, it is typically much better! The reason is that Filon-type methods are far superior for small values of n, before the onset of 'proper' asymptotic behaviour, since they exhibit high conventional order of approximation for low frequencies (Iserles 2004).

3.4 Computation without derivatives

An obvious potential shortcoming of both asymptotic and Filon-type methods is that they require the computation of derivatives of the function f. Although sometimes the data (3.10) can be computed with ease, whether directly or through automatic differentiation, this need not be the case in many relevant applications.

The current authors considered in (Iserles & Nørsett 2004) the approach of replacing derivatives with finite differences in Filon-type methods and proved that, as long as the spacing of finite differences scales inversely with frequency, asymptotic order of error decay is maintained. Similar approach can be extended to the present setting in a fairly transparent manner. The example of $s = 1$ suffices to convey the general idea. Thus, suppose again that $\boldsymbol{c}$ is given and that $\boldsymbol{m} = \mathbf{1}$: therefore we need to approximate just $f'(c_k)$, $k = 1, 2, \ldots, \nu$ from function values. Let $\delta > 0$ be a sufficiently small parameter. We approximate derivatives by finite differences, distinguishing between endpoints and internal nodes:

$$f'(-1) \approx \tfrac{1}{12}\frac{1}{\delta}[-25f(-1) + 48f(-1+\delta) - 36f(-1+2\delta) + 16f(-1+3\delta) - 3f(-1+4\delta)],$$
$$f'(c_k) \approx \tfrac{2}{3}\frac{1}{\delta}[f(c_k+\delta) - f(c_k-\delta)] - \tfrac{1}{12}\frac{1}{\delta}[f(c_k+2\delta) - f(c_k-2\delta)], \quad k = 2, \ldots, \nu-1,$$
$$f'(1) \approx \tfrac{1}{12}\frac{1}{\delta}[25f(1) - 48f(1-\delta) + 36f(1-2\delta) - 16f(1-3\delta) + 3f(1-4\delta)].$$

The above formulæ are exact for $f \in \mathbb{P}_4$, at the price of $4\nu + 2$ evaluations of the function f.

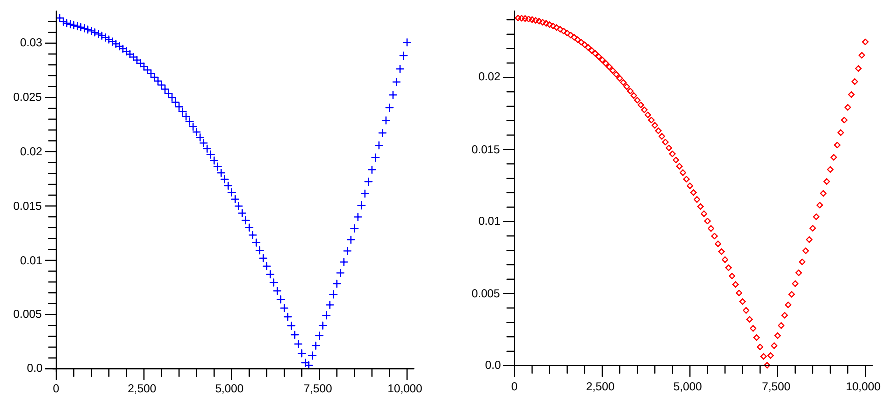

Figure 3.3: Scaled errors $n^4|\hat{A}^C_{1,n}[f] - \hat{f}^C_n|$ (on the left) and $n^4|\hat{A}^S_{1,n}[f] - \hat{f}^S_n|$, where we have replaced derivatives by finite differences with $\delta = \frac{1}{100}$, with $f(x) = \mathrm{e}^x$.

Following the discussion in (Iserles & Nørsett 2004), we need to choose δ small enough so that $m\delta < 1$ for the first m modified Fourier coefficients. In principle, this means that the method is no longer 'fully' adaptive: we need to choose m before we embark on our computation and, once we wish to compute beyond m, we need to recompute 4ν function values. Of course, we can choose δ substantially smaller than m^{-1}, where m is our initial upper bound on the number of coefficients, and this is likely to eliminate this, rather minor, snag in most cases.

As a numerical example, we have computed $\hat{A}^C_{1,n}$ and $\hat{A}^S_{1,n}$ using the above finite differences instead of derivatives, using $\delta = \frac{1}{100}$. The error matches the leftmost column of Table 1 to two significant digits. As evidenced by Fig. 3.4, the $\mathcal{O}(n^{-4})$ rate of error decay, characteristic of the original asymptotic method, remains valid up to about $n = 7200$, substantially more than δ^{-1}.

4 Conclusions

This paper is devoted to the modified Fourier expansion (1.3), its analytic features and computational aspects of the evaluation of expansion coefficients.

Insofar as the analysis of modified Fourier expansions is concerned, this is clearly an initial foray into a broad subject. Harmonic analysis, concerned with the conventional Fourier expansion (1.1) in different settings, has spawned thousands of papers and library-shelves of monographs. Needless to say, it was not our intention to replicate all this work in a modified setting in a single paper. Our more modest goal was to establish equivalent versions of few classical mainstays of harmonic analysis and explore similarities and differences with our setting.

The computation of modified Fourier coefficients follows an approach established in our previous work on Filon-type methods and highly oscillatory quadrature (Iserles & Nørsett

2004, Iserles & Nørsett 2005), but the current setting lends itself to further simplification, rationalisation and exploitation of special features to render computation even more affordable and precise. Again, we lay no claim to a complete theory. Loose ends remain and, we trust, will be the subject of future research.

Classical Fourier expansion is an immensely powerful mathematical concept and counts among the most important and fruitful techniques in applications. This paper, needless to say, neither attempts nor succeeds to replace or supersede it for the full range of its applications. Yet, it presents a technique which in specific situations confers genuine advantages over classical Fourier series and, we believe, is worthy of further study and consideration.

Acknowledgments

We wish to thank Brad Baxter (Birkbeck College), Chris Budd (University of Bath), Andy Hausrath (University of Arizona), Daan Huybrechs (Louven), Tom Körner (University of Cambridge), Peter Lindquist (NTNU Trondheim), Allan Pinkus (Technion), Alexei Shadrin (University of Cambridge), Kristian Seip (NTNU Trondheim), Divakar Viswanath (University of Michigan) and Enrique Zuazua (Universidad Autonoma, Madrid) for very useful and illuminating discussions.

References

Abramowitz, M. & Stegun, I. A., eds (1964), *Handbook of Mathematical Functions*, National Bureau of Standards, Washington, DC.

Davies, E. B. (1995), *Spectral Theory and Differential Operators*, number 42 *in* 'Cambridge Studies in Advanced Mathematics', Cambridge University Press, Cambridge.

Henrici, P. (1986), *Applied and Computational Complex Analysis*, Vol. 3, John Wiley & Sons, New York.

Huybrechs, D. & Vandewalle, S. (2006), 'On the evaluation of highly oscillatory integrals by analytic continuation', *SIAM J. Num. Anal.* To appear.

Iserles, A. (2004), 'On the numerical quadrature of highly-oscillating integrals I: Fourier transforms', *IMA J. Num. Anal.* **24**, 365–391.

Iserles, A. & Nørsett, S. P. (2004), 'On quadrature methods for highly oscillatory integrals and their implementation', *BIT* **44**, 755–772.

Iserles, A. & Nørsett, S. P. (2005), 'Efficient quadrature of highly oscillatory integrals using derivatives', *Proc. Royal Soc. A* **461**, 1383–1399.

Körner, T. W. (1988), *Fourier Analysis*, Cambridge University Press, Cambridge.

Krein, M. G. (1935), 'On a special class of differential operators', *Doklady AN USSR* **2**, 345–349.

Lorenz, G. G., Jetter, K. & Riemenschneider, S. D. (1983), *Birkhoff Interpolation*, Addison–Wesley, London.

Olver, S. (2006), ‘Moment-free numerical integration of highly oscillatory functions’, *IMA J. Num. Anal.* **26**, 213–227.

Rainville, E. D. (1960), *Special Functions*, Macmillan, New York.

Rao, K. R. & Yip, P. (1990), *Discrete Cosine Transform: Algorithms, Advantages, Applications*, Academic Press, Boston.

Young, R. M. (1980), *An Introduction to Nonharmonic Fourier Series*, Academic Press, New York.