

# 18.330 Lecture Notes: Clenshaw-Curtis Quadrature

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## 1 Newton-Cotes Quadrature

In the first unit of the course we discussed *Newton-Cotes quadrature*. Recall that this technique approximates an integral  $\int_a^b f(x) dx$  by **(1)** dividing  $[a, b]$  into  $N$  subintervals of width  $\Delta = \frac{b-a}{N}$ , **(2)** approximating  $f(x)$  by a  $p$ -th degree polynomial  $P(x)$  on each subinterval (where  $P$  is chosen to match the values of  $f$  at  $p+1$  equally spaced points in the subinterval), and then **(3)** integrating  $P(x)$  over the subinterval to approximate the integral of  $f$ . The upshot is that, for each value of  $p$ , we obtain a Newton-Cotes quadrature rule for the integral of our function. As a reminder, the rules obtained for the first three values of  $p$  are listed in the following table.

$p$	Name	Approximation to $\int_a^b f(x) dx$
0	rectangular rule	$\sum_{n=0}^{N-1} \Delta f(a + n\Delta)$
1	trapezoidal rule	$\sum_{n=0}^{N-1} \frac{\Delta}{2} \left[ f(a + n\Delta) + f(a + (n+1)\Delta) \right]$
2	Simpson's rule	$\sum_{n=0}^{N-1} \frac{\Delta}{6} \left[ f(a + n\Delta) + 4f\left(a + \left(n + \frac{1}{2}\right)\Delta\right) + f(a + (n+1)\Delta) \right]$

When we discussed Newton-Cotes quadrature previously, we offered the following heuristic convergence analysis: The  $p$ -th order NC rule models  $f$  as a  $p$ -th degree polynomial, which means the error in the approximation is a polynomial that starts at degree  $p+1$ . The integral of this error polynomial over an interval of width  $\Delta$  is proportional to  $\Delta^{p+2} \sim \frac{1}{N^{p+2}}$ . Hence the error in our approximate estimate of the integral *over each subinterval* is

$$\text{error per subinterval} \sim \frac{1}{N^{p+2}}$$

and there are  $N$  subintervals, so

$$\text{total error} = N \cdot (\text{error per subinterval}) \sim \frac{1}{N^{p+1}}. \quad (1)$$

In other words, our heuristic convergence analysis suggests that the error should decay algebraically with  $N$ , with faster decay for larger values of  $p$ . However, this analysis is clearly oversimplified – in particular, equation (1) blindly sums the errors within each subinterval, without considering the possibility of *cancellations* among the errors in different subinterval.

When you investigated the performance of NC quadrature rules in PSet 1, you found that the heuristic prediction (1) is actually borne out in practice on a fairly wide class of functions, but with some glaring exceptions. In particular, although the error incurred by the rectangular and trapezoidal rules did indeed decay respectively like  $\sim \frac{1}{N}$  and  $\sim \frac{1}{N^2}$  for most functions, in some special cases—namely, for periodic functions integrated over their period or an integer multiple of their period—the error seemed to be decaying *exponentially* rapidly with  $N$ . There is nothing in our heuristic convergence analysis that could possibly explain this phenomenon.

But now that we are equipped with the tools of Fourier analysis, we can obtain understand this phenomenon in more detail – and, in the process, learn how the excellent behavior of Newton-Cotes quadrature for periodic functions can be recovered for non-periodic functions as well. This will lead us to the numerical integration technique known as *Clenshaw-Curtis quadrature*.

## 2 Fourier-Series Convergence Analysis of the Trapezoidal Rule

Let's consider the integral of a function  $f(t)$  over an interval of width  $T$ , which we assume without loss of generality to start at  $t = 0$ . Thus we are trying to compute

$$\mathcal{I} = \int_0^T f(t) dt.$$

The  $N$ -point trapezoidal-rule approximation to  $\mathcal{I}$  is

$$I_N^{\text{trap}} = \frac{T}{N} \left\{ \frac{1}{2} [f(0) + f(T)] + \sum_{n=1}^{N-1} f\left(\frac{nT}{N}\right) \right\}. \quad (2)$$

This formula is just the second box of the table in the previous section, with  $a = 0$ ,  $b = T$ , and  $\Delta = \frac{T}{N}$ . What we would like to understand is the  $N$  dependence of the error

$$\mathcal{E}_N^{\text{trap}} = |\mathcal{I} - I_N^{\text{trap}}|.$$

To do this, recall from our discussion of Fourier analysis that our function may be represented over the interval  $[0, T]$  in the form

$$f(t) = \sum_{\nu=-\infty}^{\infty} \tilde{f}_{\nu} e^{i\nu\omega_0 t} \quad \left( \omega_0 = \frac{2\pi}{T} \right) \quad (3)$$

where the Fourier series coefficients are

$$\tilde{f}_{\nu} = \frac{1}{T} \int_0^T f(t) e^{-i\nu\omega_0 t} dt. \quad (4)$$

In particular, the integral we are trying to compute is precisely just  $T$  times the value of the  $\nu = 0$  Fourier series coefficient:

$$\mathcal{I} = T \tilde{f}_0.$$

Of course, when we are doing Newton-Cotes quadrature on a function  $f(t)$  we don't *know* its Fourier series coefficients—if we did, we wouldn't need to be doing quadrature in the first place—but the point is that even without knowing the values of the  $\tilde{f}_{\nu}$  we know that the Fourier-synthesized representation (3) exists, and that is all that we need for this analysis.

We now want to insert the representation (3) into (2). Conveniently, the first term on the RHS of (2) is precisely what we get by evaluating the Fourier series (3) at  $t = 0$ .<sup>1</sup> For the other terms, we simply plug in equation (3) evaluated at

<sup>1</sup>This is obviously true when the original function  $f(t)$  is periodic with period  $T$ , but when  $f(0) \neq f(T)$  it is a non-trivial and convenient fact that the first term on the RHS of (2) is precisely what we get by evaluating the Fourier series (3) at  $t = 0$ . This, incidentally, is the reason for starting with a convergence analysis of the trapezoidal rule instead of the rectangular rule; the latter can be analyzed using Fourier-series techniques as well, but the analysis is not as nice.

various different values of the argument  $t$ :

$$\begin{aligned}
 I_N^{\text{trap}} &= \frac{T}{N} \left\{ \underbrace{\frac{1}{2}[f(0) + f(T)]}_{\sum \tilde{f}_m} + \sum_{n=1}^{N-1} \underbrace{f\left(\frac{nT}{N}\right)}_{\sum \tilde{f}_m e^{im\omega_0(\frac{nT}{N})}} \right\} \\
 &= \frac{T}{N} \sum_{n=0}^{N-1} \left\{ \sum_{\nu=-\infty}^{\infty} \tilde{f}_\nu e^{i\nu\omega_0(\frac{nT}{N})} \right\} \\
 &= \frac{T}{N} \sum_{n=0}^{N-1} \left\{ \sum_{\nu=-\infty}^{\infty} \tilde{f}_\nu e^{2\pi i m n / N} \right\} \tag{5}
 \end{aligned}$$

where I used  $\omega_0 = \frac{2\pi}{T}$ . Now rearrange the sums:

$$= T \sum_{\nu=-\infty}^{\infty} \tilde{f}_\nu \underbrace{\left\{ \frac{1}{N} \sum_{n=0}^{N-1} e^{2\pi i \nu n / N} \right\}}_{K_N(\nu)} \tag{6}$$

In the last line here we defined a function  $K_N(\nu)$  which has some interesting properties:

$$\begin{aligned}
 K_N(\nu) &= \frac{1}{N} \sum_{n=0}^{N-1} e^{2\pi i \nu n / N} \\
 &= \frac{1}{N} [1 + \zeta + \zeta^2 + \cdots + \zeta^{N-1}] \tag{7}
 \end{aligned}$$

where  $\zeta = e^{2\pi i \nu / N}$ . Now, if  $\nu = 0$  or  $\nu$  is an integer multiple of  $N$ , then  $\zeta = 1$  and the sum simply yields

$$K_N(\nu) = 1 \quad \text{if } \nu \text{ is an integer multiple of } N$$

On the other hand, if  $\nu$  is not an integer multiple of  $N$ , then  $\zeta \neq 1$  in (7) and we may sum the geometric series to find

$$\begin{aligned}
 K_N(\nu) &= \frac{1}{N} \left[ \frac{1 - \zeta^N}{1 - \zeta} \right] \\
 &= \frac{1}{N} \left[ \frac{1 - e^{2\pi i \nu}}{1 - e^{2\pi i \nu / N}} \right] \\
 &= 0 \quad \text{if } \nu \text{ is not an integer multiple of } N.
 \end{aligned}$$

Now going back to (6), we find that the sum over Fourier coefficients is now restricted to  $\nu$  values that are integer multiples of  $N$ ,  $\nu = pN$  with  $p \in \mathbb{Z}$ :

$$I_N^{\text{trap}} = T \sum_p \tilde{f}_{pN}.$$

So the  $N$ -point trapezoidal-rule approximation to the integral of  $f$  is picking out precisely just the Fourier-series coefficients with frequencies that are multiples of  $N\omega_0$ . In particular, the  $\nu = 0$  term here is the exact integral  $\mathcal{I}$  that we are seeking, and everything else is an error term:

$$I_N^{\text{trap}} = \underbrace{T\tilde{f}_0}_{\mathcal{I}} + T \sum_{p \neq 0} \tilde{f}_{pN}.$$

Thus the error  $\mathcal{E}_N^{\text{trap}} = |\mathcal{I} - I_N^{\text{trap}}|$  is just the sum of the  $\pm N$ th,  $\pm 2N$ th, etc. Fourier-series coefficients of our function:

$$\mathcal{E}_N^{\text{trap}} = \left| \sum_{\substack{p=-\infty \\ p \neq 0}}^{\infty} \tilde{f}_{pN} \right|. \quad (8)$$

Of course, again, we don't know the numbers  $\tilde{f}_{pN}$ , so we can't compute the RHS of this formula exactly. However, we can use the smoothness-vs.-decay properties of Fourier analysis to estimate how rapidly it decays with  $N$ .

### Convergence for continuous nonperiodic functions $f(t)$

First suppose  $f(t)$  is a continuous function that does not satisfy the condition  $f(0) = f(T)$ , i.e.  $f(t)$  takes different values at the endpoints of the interval over which we are integrating. In this case, the Fourier-series coefficients we compute using equation (4) are really the Fourier-series coefficients of a *discontinuous* function  $f^{\text{per}}(t)$  obtained by slicing out just the portion of  $f(t)$  between 0 and  $T$  and periodically repeating it, as illustrated in Figure 1. [ $f^{\text{per}}(t)$  is sometimes known as the  *$T$ -periodic extension* of  $f(t)$ . We might refer to it as the “brute-force” periodic extension of  $f(t)$ ; this is in contrast to the more elegant way to define a periodic extension of  $f(t)$  that we consider later.] From general Paley-Wiener analysis we know that, for a discontinuous function, the magnitudes of the Fourier series coefficients  $|\tilde{f}_\nu|$  decay like  $|\tilde{f}_\nu| \sim 1/\nu$ , and hence looking at (8) we might expect that the error in the trapezoidal rule should decay like  $1/N$ .

However, this point turns out to require more careful scrutiny, because the error formula (8) actually involves the sum of Fourier coefficients  $\tilde{f}_\nu$  corresponding to both positive and negative values of  $\nu$ , and this turns out to yield a curious cancellation. The full calculation is performed in Appendix A, but the long story short is that the Fourier-series coefficient  $\tilde{f}_\nu$  may be expressed as a power series in inverse powers of  $\nu$ :

$$\tilde{f}_\nu = \frac{C_1}{\nu} + \frac{C_2}{\nu^2} + \frac{C_3}{\nu^3} + \frac{C_4}{\nu^4} + \dots \quad (9)$$

This means that, when we compute the pairwise sum of positive-index and negative-index Fourier coefficients, the terms with odd powers of  $\nu$  have opposite signs and thus *cancel* out of sum, leaving only even powers of  $\nu$ :

$$\tilde{f}_\nu + \tilde{f}_{-\nu} = \frac{C'_2}{\nu^2} + \frac{C'_4}{\nu^4} + \dots$$

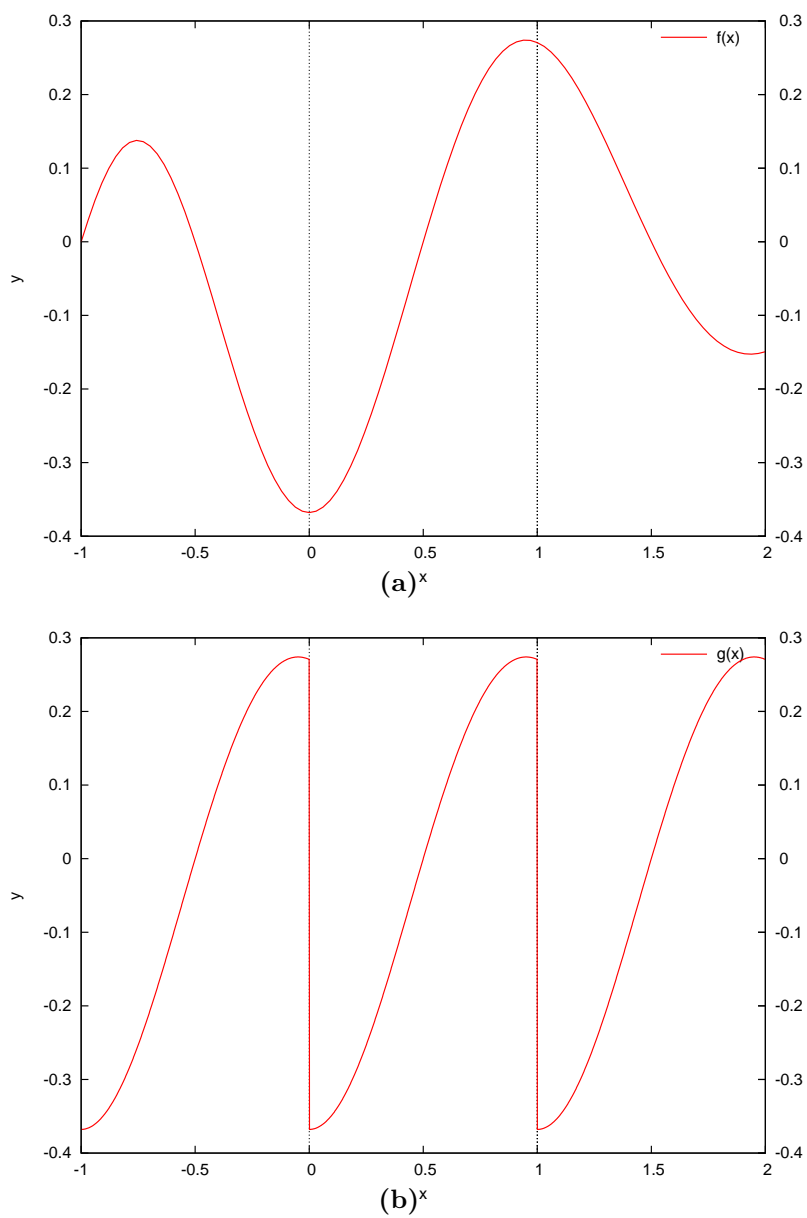


Figure 1: **(a)** A non-periodic function that we might be trying to integrate over the interval  $[0, 1]$ . **(b)** The actual function whose Fourier-series coefficients we are computing when we evaluate equation (4). Note that this function is discontinuous even though the original function was continuous.

(Here I have put  $C'_\nu = 2C_\nu$ ; the constant prefactors aren't as important here as the asymptotic behavior with respect to  $\nu$ .) Thus the terms proportional to  $1/N$  cancel out of (8), and we have

$$\begin{aligned}\mathcal{E}_N^{\text{trap}} &= \left| \sum_{p=1}^{\infty} \left( \tilde{f}_{pN} + \tilde{f}_{-pN} \right) \right| \\ &= \left| \sum_{p=1}^{\infty} \left( \frac{C'_2}{pN^2} \right) \right| \\ &= \frac{C'_2}{N^2} \underbrace{\sum_{p=1}^{\infty} \frac{1}{p^2}}_{\pi^2/6}\end{aligned}$$

Where have we seen this sum over  $p$  before? The fact that the sum over  $p$  may be evaluated in closed form is nice, but somewhat irrelevant for our purposes; the only thing that's important is that the overall error decays like  $N^2$ , i.e.

$$\mathcal{E}_N^{\text{trap}} \sim \frac{1}{N^2}.$$

So there's the  $1/N^2$  convergence of the trapezoidal rule.

### Convergence for periodic functions $f(t)$

On the other hand, suppose that our original function  $f(t)$  was not only smooth but also *periodic* with period  $T$ . This means not only that  $f(0) = f(T)$ , but also that  $f'(0) = f'(T)$ ,  $f''(0) = f''(T)$ , and all higher derivatives agree at the endpoints. In this case the function whose Fourier series we are computing is  $C^\infty$ , and we know from the general Paley-Wiener theorem of Fourier analysis that the magnitudes of its Fourier coefficients  $|\tilde{f}_\nu|$  decay *faster than any polynomial* in  $\nu$ , with behavior like  $|\tilde{f}_N| \sim e^{-\alpha|N|}$  typical. In such a case we find

$$\begin{aligned}\mathcal{E}_N^{\text{trap}} &= \left| \sum_{p \neq 0} \tilde{f}_{pN} \right| \\ &= \left| \sum_{p \neq 0} e^{-\alpha N|p|} \right|\end{aligned}$$

and the sum will be dominated by its first terms,

$$\sim e^{-\alpha N}.$$

This explains the exponential convergence rate of the trapezoidal rule applied to periodic functions.



### 3 Clenshaw-Curtis Quadrature

The discussion of the previous section explains why the simple trapezoidal rule converges so rapidly for periodic functions, and why it converges relatively *slowly* for non-periodic functions. Thus, if we are lucky enough to be integrating a periodic function over a period, all we have to do is apply the usual trapezoidal rule and we magically get exponential convergence. But what if we have the bad fortune of needing to integrate a non-periodic function? Are we stuck with the slow convergence of the trapezoidal rule?

No! This is actually a general principle of mathematics, and of life more broadly: *You are not helpless. You have options.* In particular, in the case at hand we have the option to *convert* our non-periodic function into a periodic function, and the process of availing ourselves of this option is known as *Clenshaw-Curtis quadrature*.

#### Constructing a periodic function $g$ from our non-periodic function $f$

Clenshaw-Curtis quadrature is nicest to formulate when the interval over which we are trying to integrate our function is  $[-1, 1]$ , so we will consider that case here.<sup>2</sup> Thus consider the integral

$$\mathcal{I} = \int_{-1}^1 f(t) dt. \quad (10)$$

The interval  $[-1, 1]$  happens to be precisely the range of values covered (though not in the same order) by  $\cos \theta$  as  $\theta$  ranges from  $0$  to  $\pi$ , so it is convenient to use the parameterization  $t = \cos \theta$  and to define a new function

$$g(\theta) \equiv f(\cos \theta). \quad (11)$$

Figure 2 shows some non-periodic function  $f(t)$  together with the function  $g(\theta) \equiv f(\cos \theta)$ . Notice the following points about  $g(\theta)$  :

- (a) It is a periodic function with period  $T = 2\pi$ .
- (b) It is an even function, i.e.  $g(-\theta) = g(\theta)$ .
- (c) As  $\theta$  ranges from  $0 \rightarrow \pi$ ,  $g(\theta)$  traces out the behavior of  $f(t)$  as  $t$  ranges *backward* from  $1 \rightarrow -1$ .
- (d)  $g(\theta)$  knows nothing about the behavior of  $f(t)$  outside the range  $-1 \leq t \leq 1$ . This can make it a little tricky to compare the two plots. For example,  $g(\theta)$  has local minima at  $\theta = 0, \pi$  even though  $f(t)$  does not have local minima at  $t = 1, -1$ .

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<sup>2</sup>If you need to integrate a function  $f(t)$  over some other interval  $[a, b]$ , just define  $g(u) = f\left(a + \frac{(b-a)}{2}(u+1)\right)$  and apply Clenshaw-Curtis quadrature to integrate  $g(u)$  from  $u = -1$  to  $1$ . Don't forget the Jacobian factor.

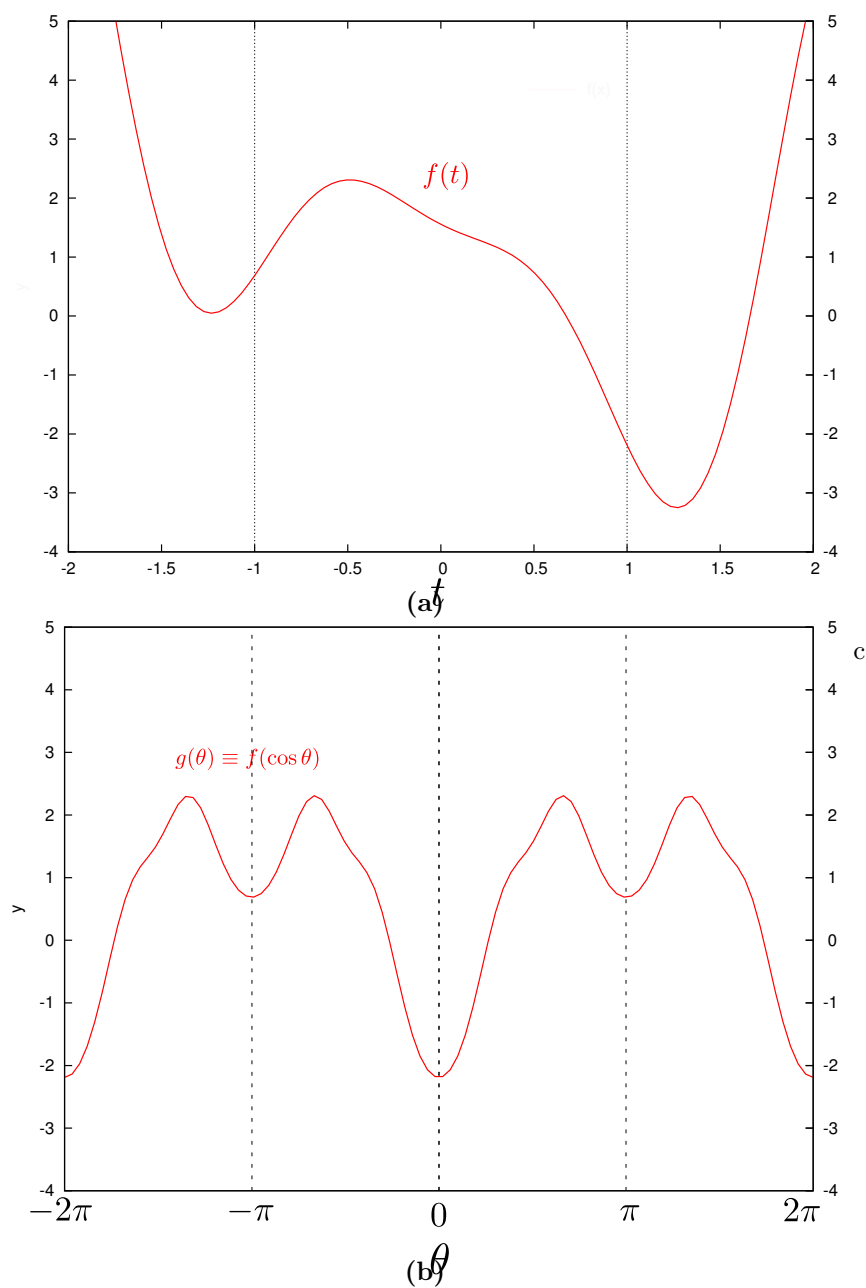


Figure 2: **(a)** A function  $f(t)$  that we want to integrate over the interval  $[-1, 1]$ . **(b)** The function  $g(\theta) = f(\cos \theta)$ . Note the following facts: **(1)**  $g(\theta)$  is periodic with period  $2\pi$ . **(2)**  $g(\theta)$  is an even function of  $\theta$ . **(3)** Over the interval  $0 \leq \theta \leq \pi$ ,  $g(\theta)$  reproduces the behavior of  $f(t)$ . However, **(4)**  $g(\theta)$  knows *nothing* about what  $f(t)$  does outside the range  $-1 < t < 1$ , which can make it a little tricky to compare the two plots. For example,  $g(\theta)$  has local minima at  $\theta = 0, \pi$  even though  $f(t)$  does not have local minima at  $t = 1, -1$ .

Property **(a)** here ensures that the function  $g(\theta)$  has a Fourier-series representation involving sinusoids that are integer multiples of a base period  $\omega_0 = \frac{2\pi}{T} = 1$ :

$$g(\theta) = \sum_{\nu=-\infty}^{\infty} \tilde{g}_{\nu} e^{i\nu\theta}, \quad \tilde{g}_{\nu} = \frac{1}{2\pi} \int_0^{2\pi} g(\theta) e^{-i\nu\theta} d\theta. \quad (12)$$

Meanwhile, property **(b)** ensures that this Fourier series contains only cosine terms, i.e. it is a *Fourier cosine series*:

$$g(\theta) = \frac{\tilde{a}_0}{2} + \sum_{\nu=1}^{\infty} \tilde{a}_{\nu} \cos \nu\theta \quad (13)$$

where the  $\tilde{a}_{\nu}$  coefficients are related to the  $\tilde{g}_{\nu}$  coefficients in (12) according to

$$\tilde{a}_0 = 2\tilde{g}_0, \quad \tilde{a}_{\nu} = (\tilde{g}_{\nu} + \tilde{g}_{-\nu}) = 2\tilde{g}_{\nu} \quad (14)$$

(where we used the fact that the Fourier-series coefficients of an even real-valued function satisfy  $\tilde{g}_{\nu} = \tilde{g}_{-\nu}$ ). The  $\tilde{a}$  coefficients may also be written in the form

$$\tilde{a}_{\nu} = \frac{1}{\pi} \int_0^{2\pi} g(\theta) \cos(\nu\theta) d\theta. \quad (15)$$

Notice something very important about these integrals: They are integrals of a periodic function over its period. (Indeed, both  $g(\theta)$  and  $\cos(\nu\theta)$  for integer  $\nu$  are periodic functions over the interval  $[0 : 2\pi]$ , so the whole integrand is periodic.) That means the integral (15) can be evaluated using a simple  $N$ -point trapezoidal rule with an error that decays *exponentially* with  $N$ .

### The integral of $f$ in terms of the Fourier-series coefficients

We now want to rewrite our integral (10) in terms of our newly-constructed periodic function  $g$ . To do this, we simply change variables in (10) according to  $t = \cos \theta$ :

$$\begin{aligned} \mathcal{I} &= \int_{-1}^1 f(t) dt = \int_0^{\pi} f(\cos \theta) \sin \theta d\theta \\ &= \int_0^{\pi} g(\theta) \sin \theta d\theta. \end{aligned} \quad (16)$$

Although  $g(\theta)$  is a periodic function, we don't obtain an exponentially-convergent quadrature rule by applying the trapezoidal rule directly to (16) because the range of integration is only over *half* the period of the integrand (the integral runs from 0 to  $\pi$ , whereas the period of the integrand is  $2\pi$ ). However, something brilliant happens when we plug in the Fourier-cosine-series representation of  $g(\theta)$ :

$$\begin{aligned} \mathcal{I} &= \int_0^{\pi} g(\theta) \sin \theta d\theta \\ &= \int_0^{\pi} \left\{ \frac{\tilde{a}_0}{2} + \sum_{\nu=1}^{\infty} \tilde{a}_{\nu} \cos(\nu\theta) \right\} \sin \theta d\theta \end{aligned}$$

Rearrange the sum and evaluate the integral:

$$\mathcal{I} = \underbrace{\frac{\tilde{a}_0}{2} \int_0^\pi \sin \theta d\theta}_2 + \sum_{\nu=0}^{\infty} a_\nu \underbrace{\left\{ \int_0^\pi \cos(\nu\theta) \sin \theta d\theta \right\}}_{\frac{1+(-1)^\nu}{1-\nu^2}} \quad (17)$$

The integral vanishes if  $\nu$  is odd, and yields  $2/(1-\nu^2)$  if  $\nu$  is even, so we find simply

$$\mathcal{I} = \tilde{a}_0 + \sum_{\substack{\nu=1 \\ \nu \text{ even}}}^{\infty} \frac{2\tilde{a}_\nu}{1-\nu^2}. \quad (18)$$

Equation (18) expresses the integral of our function  $f(t)$  in terms of the Fourier-cosine-series coefficients of  $g(\theta)$ , defined by equation (15).

Moreover, the sum in (18) is rapidly convergent, because (assuming the original function  $f$  is a smooth function) the function  $g(\theta)$  is smooth and *periodic*, so its Fourier-cosine-series coefficients  $\tilde{a}_\nu$  decay faster than any polynomial in  $\nu$ . (Note that this would *not* be the case if we had simply constructed a brute-force periodic extension of  $f(t)$  by slicing out its behavior between  $[-1 : 1]$  and periodically repeating it; in that case the function would have discontinuities at the endpoints of the interval and its Fourier coefficients would only decay algebraically with  $\nu$ .)

Hence, in practice, we can truncate the sum in (18) at some finite number of terms, i.e. we keep terms up to  $a_N$  for some even integer  $N$ , which then defines the Clenshaw-Curtis approximation to our integral:<sup>3</sup>

$$\mathcal{I} \approx I_N^{\text{CC}} \equiv \tilde{a}_0 + \sum_{\substack{\nu=1 \\ \nu \text{ even}}}^N \frac{2\tilde{a}_\nu}{1-\nu^2}. \quad (19)$$

For reasons that will become apparent shortly, it is convenient to think of the cosine-series coefficients  $\tilde{a}_\nu$  as the elements of an  $(N+1)$ -dimensional vector  $\tilde{\mathbf{a}}$ , and to think of equation (19) as the dot product of this vector with a weight vector  $\mathbf{W}$  whose elements are just the coefficients of  $a_\nu$  in the sum (18):

$$\mathcal{I} = \mathbf{W} \cdot \tilde{\mathbf{a}} \quad (20)$$

where

$$\tilde{\mathbf{a}} = \begin{pmatrix} \tilde{a}_0 \\ \tilde{a}_1 \\ \vdots \\ \tilde{a}_N \end{pmatrix} \quad \mathbf{W} = \begin{pmatrix} W_0 \\ W_1 \\ \vdots \\ W_N \end{pmatrix}, \quad W_\nu \equiv \begin{cases} 1, & \nu = 0 \\ \frac{2}{1-\nu^2}, & \nu \neq 0 \text{ even} \\ 0, & \nu \text{ odd} \end{cases}$$

<sup>3</sup>Some authors weight the last term in this sum (i.e. the term involving  $a_N$ ) with a factor of  $1/2$ . There are theoretical reasons for doing this, but we won't bother with this complication here; in any event that term is exponentially suppressed relative to the other terms in the sum, so its prefactor doesn't matter much.

## Two ways to proceed

Having derived equation (19), there are now two directions in which we could proceed to compute numerical integrals.

- We could approximate the Fourier-coefficient integral, equation (15), using an  $N$ -point trapezoidal rule.<sup>4</sup> Since this is an integral of a periodic function over its period, the error in this procedure will decrease exponentially<sup>5</sup> with  $N$ . Moreover, the trapezoidal-rule approximation to  $\tilde{a}_\nu$  will sample  $g(\theta) = f(\cos \theta)$  at the *same*  $N$  points for all values of  $\nu$ , and (19) then amounts to a weighted sum over those function samples—that is, it amounts to an  $N$ -point quadrature rule.
- Alternatively, we could approximate the  $\tilde{a}_\nu$  coefficients using a fast Fourier transform and evaluate the sum (19) directly.

Both of these viewpoints are useful in practice. We will consider the first of these possibilities in the next section, and the second possibility in our lecture notes on discrete Fourier transforms.

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<sup>4</sup>Actually we could use any  $M$ -point trapezoidal rule here with  $M$  not necessarily having any particular relationship to  $N$ ; in this case the error in the individual coefficients would decay like  $e^{-\#M}$  while the error in the sum (19) would decay like  $e^{-\#N}$ , and the overall error would be determined by the smaller of the two.

<sup>5</sup>Technically, the proper statement is that the error will decrease faster than any polynomial in  $N$ , which still leaves open the possibility of convergence like  $e^{-\sqrt{N}}$ , which is faster than any polynomial but not exponentially fast. We are only guaranteed to get exponential convergence if the original function  $f(t)$  is analytic.

## 4 Clenshaw-Curtis Quadrature Rules

Equation (19) expresses the Clenshaw-Curtis approximation to the integral  $\mathcal{I}$  in terms of the numbers  $\tilde{a}_\nu$ , the Fourier-cosine-series coefficients of the function  $g(\theta) \equiv f(\cos \theta)$ . To turn this into a usual quadrature rule, we just need to express those coefficients in terms of samples of the function  $f$ .

### Expressing $\tilde{a}_\nu$ in terms of samples of $f(t)$

But this is easy to do. Recall from equations (11), (12), (14), and (15) that the  $\tilde{a}_\nu$  coefficients are defined by

$$\tilde{a}_\nu = \frac{1}{\pi} \int_0^{2\pi} f(\cos \theta) \cos(\nu \theta) d\theta.$$

Because this is the integral of a periodic function over a period, we can estimate it using the simple trapezoidal rule, with error decaying exponentially rapidly<sup>6</sup> with the number of sample points. Actually, because the integrand is an even function of  $\theta$ , we can integrate over just half the integration range and double the result:

$$\tilde{a}_\nu = \frac{2}{\pi} \int_0^\pi f(\cos \theta) \cos(\nu \theta) d\theta$$

Apply an  $N$ -subinterval trapezoidal rule:

$$\approx \frac{2}{N} \sum'_{n=0} f(\cos \theta_n) \cos(\nu \theta_n) \quad (21)$$

where the primed sum indicates that the first and last terms are to be weighted by a factor of  $1/2$ , and where

$$\theta_n \equiv \frac{n\pi}{N}.$$

Introducing some convenient shorthand notation, we can write equation (21) in the form

$$\tilde{a}_\nu = \sum_n \Lambda_{\nu n} f(t_n) \quad (22)$$

---

<sup>6</sup>The usual caveats apply: **(1)** We only get this rapid convergence behavior if the original function  $f(t)$  is smooth; the Clenshaw-Curtis periodization algorithm (11) smooths out the discontinuity at the *endpoints* that would be caused by brute-force periodization, but doesn't smooth out any other bad behavior in  $f(t)$ . **(2)** Technically, the smoothness of  $f$  only guarantees convergence faster than any polynomial in  $N$ ; we can only make the stronger prediction of *exponential* convergence if  $f$  is also *analytic* (i.e. has a convergent Taylor series at each point in the domain of interest). In practical numerical work the distinction between smooth and analytic functions is rarely important, so it is typically safe to expect errors that decay exponentially with  $N$ .

where

$$t_n \equiv \cos \frac{\pi n}{N}, \quad \Lambda_{\nu n} \equiv \begin{cases} \frac{1}{N} \cos \left( \frac{n\nu\pi}{N} \right), & n = 0 \\ \frac{2}{N} \cos \left( \frac{n\nu\pi}{N} \right), & n = 1, 2, \dots, N-1 \\ \frac{1}{N} \cos \left( \frac{n\nu\pi}{N} \right), & n = N. \end{cases}$$

The points  $t_n \equiv \cos \frac{\pi n}{N}, n = 0, \dots, N$  are called *Chebyshev points*, and we will have more to say about them later. For the time being, the important thing about equation (22) is that we are sampling  $f$  at the *same* quadrature points to compute the values of each of the various  $\tilde{a}_\nu$  coefficients. This means that equation (22) may be written in the form of a matrix equation:

$$\tilde{\mathbf{a}} = \mathbf{\Lambda} \mathbf{f} \quad (23)$$

where  $\tilde{\mathbf{a}}$  is the length- $(N+1)$  vector of  $\tilde{a}_\nu$  coefficients,  $\mathbf{\Lambda}$  is the  $(N+1) \times (N+1)$  matrix of  $\Lambda_{\nu n}$  coefficients, and  $\mathbf{f}$  is the length- $(N+1)$  vector of samples of  $f$ :

$$\tilde{\mathbf{a}} = \begin{pmatrix} \tilde{a}_0 \\ \tilde{a}_1 \\ \vdots \\ \tilde{a}_N \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f(t_0) \\ f(t_1) \\ \vdots \\ f(t_N) \end{pmatrix}, \quad t_n \equiv \frac{\pi n}{N}.$$

$$\mathbf{\Lambda} = \frac{2}{N} \begin{pmatrix} \frac{1}{2} & 1 & 1 & 1 & 1 & \frac{1}{2} \\ \frac{1}{2} & \cos \frac{\pi}{N} & \cos \frac{2\pi}{N} & \cos \frac{3\pi}{N} & \dots & \frac{1}{2} \cos \pi \\ \frac{1}{2} & \cos \frac{2\pi}{N} & \cos \frac{4\pi}{N} & \cos \frac{6\pi}{N} & \dots & \frac{1}{2} \cos 2\pi \\ \frac{1}{2} & \cos \frac{3\pi}{N} & \cos \frac{6\pi}{N} & \cos \frac{9\pi}{N} & \dots & \frac{1}{2} \cos 3\pi \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2} & \cos \pi & \cos 2\pi & \cos 3\pi & \dots & \frac{1}{2} \cos N\pi \end{pmatrix} \quad (24)$$

### Expressing $\mathcal{I}$ in terms of samples of $f$ :

Equation (20) expresses our desired integral  $\mathcal{I}$  in terms of the  $\tilde{a}_\nu$  coefficients, while equation (23) expresses the  $\tilde{a}_\nu$  coefficients in terms of samples of  $f$  at the Chebyshev points. Thus, combining the two equations yields an expression for  $\mathcal{I}$  in terms of samples of  $f$ —that is, a quadrature rule:

$$\mathcal{I} = \mathbf{W}^T \mathbf{\Lambda} \mathbf{f}$$

or

$$\mathcal{I} = \mathbf{w} \cdot \mathbf{f} \quad (25)$$

where  $\mathbf{w}$  is just the  $(N + 1)$ -dimensional vector obtained by multiplying the vector  $\mathbf{W}$  by the transpose<sup>7</sup> of the matrix  $\mathbf{\Lambda}$ :

$$\mathbf{w} \equiv \mathbf{\Lambda}^T \mathbf{W}.$$

Writing out equation (25), we have

$$\mathcal{I} = \int_{-1}^1 f(t) dt = \sum_{n=0}^N w_n f(t_n)$$

This is nothing but an  $(N + 1)$ -point quadrature rule expressing the integral  $\mathcal{I}$  as a weighted sum of samples of  $f$ .

Thus, to construct the vector of weights  $\mathbf{w}$  in a Clenshaw-Curtis quadrature rule, we simply

1. form the vector  $\mathbf{W}$  defined by equation (20),
2. form the matrix  $\mathbf{\Lambda}$  defined by equation (24),
3. set  $\mathbf{w}$  as the matrix-vector product:  $\mathbf{w} = \mathbf{\Lambda}^T \mathbf{W}$ .

### Clenshaw-Curtis quadrature rules for $N = 4$ and $N = 5$

Just to be explicit, here are numerical tables of the points and weights for the Clenshaw-Curtis quadrature rules for  $N = 4$  and  $N = 5$ . (Note that the rule for a given value of  $N$  contains  $N + 1$  points.)

$N = 4$

$n$	$t_n$	$w_n$
0	1.0	0.05
1	0.707107	0.566667
2	0.0	0.766667
3	-0.707107	0.566667
4	-1.0	0.05

$N = 5$

$n$	$t_n$	$w_n$
0	1.0	0.04
1	0.809017	0.360743
2	0.309017	0.599257
3	-0.309017	0.599257
4	-0.809017	0.360743
5	-1.0	0.04

A good first way to test a code for computing the weights  $w_n$  is to check that they all sum to 2, i.e.  $\sum_{n=0}^N w_n = 2$ . (This corresponds to integrating the function  $f(t) = 1$  over the interval  $[-1, 1]$ .)

<sup>7</sup>The transpose of a matrix can be obtained in JULIA and MATLAB by appending a single quote (') to the name of the matrix. For example, if your code contains a matrix named `Lambda` and you wish to multiply a vector `W` by the transpose of this matrix, say `Lambda' * W`.



### Explicit form of the Clenshaw-Curtis quadrature rule

For some purposes it is convenient to have an explicit formula for the weights in the Clenshaw-Curtis quadrature rule. For *even* values of  $N$ , such a formula is:

**For *even* values of  $N$ :**

$$w_m = \begin{cases} \frac{1}{N^2 - 1}, & m = 0 \\ \frac{2}{N} \left[ 1 + \left\{ \sum_{n=1}^{N/2-1} \left( \frac{2}{1 - 4n^2} \right) \cos \left( \frac{2mn\pi}{N} \right) \right\} + \frac{\cos m\pi}{1 - N^2} \right], & m = 1, \dots, N - 1 \\ \frac{1}{N^2 - 1}, & m = N. \end{cases}$$

## A Proof of equation (9)

In our Fourier-series analysis of the convergence of trapezoidal-rule quadrature, we invoked without proof the statement that the Fourier-series coefficients of a function  $f(t)$ —where  $f$  is smooth but not necessarily periodic over the period  $T$  of the Fourier series—may be expanded in inverse powers of  $\nu$ :

$$\tilde{f}_\nu = \frac{C_1}{\nu} + \frac{C_2}{\nu^2} + \frac{C_3}{\nu^3} + \frac{C_4}{\nu^4} + \cdots \quad (26)$$

This turns out to be fairly easy to establish. The trick is simply to write down the integral that defines  $\tilde{f}_\nu$ , then integrate by parts:

$$\begin{aligned} \tilde{f}_\nu &= \frac{1}{T} \int_0^T f(t) e^{-i\nu\omega_0 t} dt \\ &= \frac{1}{T} \left\{ \frac{1}{i\nu\omega_0} \underbrace{\left| f(t) e^{-i\nu\omega_0 t} \right|_0^T}_{\Delta f} + \frac{1}{i\nu\omega_0} \int_0^T f'(t) e^{-i\nu\omega_0 t} dt \right\} \end{aligned}$$

In the first term, the exponential factor evaluates to 1 at both endpoints of the interval, so we get just  $f(T) - f(0) \equiv \Delta f$  (where I have introduced the notation  $\Delta f$  as a convenient shorthand). So we find

$$\tilde{f}_\nu = \frac{\Delta f}{i\nu\omega_0 T} + \frac{1}{i\nu\omega_0} \int_0^T f'(t) e^{-i\nu\omega_0 t} dt$$

Now integrate by parts again and proceed similarly to write:

$$\tilde{f}_\nu = \frac{\Delta f}{i\nu\omega_0 T} + \frac{\Delta f'}{(i\nu\omega_0)^2} + \frac{1}{(i\nu\omega_0)^2} \int_0^T f''(t) e^{-i\nu\omega_0 t} dt$$

where  $\Delta f' \equiv f'(T) - f'(0)$ . Thus we have derived the first two terms in the expansion (26), and proceeding similarly yields the remaining terms in the sum.

Incidentally, this calculation also serves as a proof of the Paley-Wiener theorem in the Fourier-series case: If  $\Delta f=0$  but  $\Delta f' \neq 0$ , then the brute-force periodic extension of  $f(t)$  has continuous value but discontinuous derivative, so its index of discontinuity is  $p = 1$ ; the above expansion then predicts that  $|\tilde{f}_\nu| \sim 1/\nu^2$  as  $|\nu| \rightarrow \infty$ , which is just what the Paley-Wiener theorem predicts.

For more detail on this calculation see J. P. Boyd, *Chebyshev and Fourier Spectral Methods*, Section 2.9.