Ulli Wolff, Masy 2012, background material for CP1.

1 Perfect trapezoidal integrator for periodic analytic functions

In CP1 it was experimentally found the approximation

$$T_N(f) = h\left(\frac{1}{2}f_0 + f_1 + f_2 + \ldots + f_{N-1} + \frac{1}{2}f_N\right) \approx \frac{1}{2}I_0(\beta) \tag{1}$$

with[1]

$$h = \frac{\pi}{N}, \quad x_i = i\,h, \quad f_i \equiv f(x_i), \quad f(x) = \frac{1}{2\pi}\mathrm{e}^{\beta\cos(x)}$$

approximates the Bessel function

$$I_0(\beta) = \int_0^{\pi} \frac{d\varphi}{\pi}\,\mathrm{e}^{\beta\cos(\varphi)} = \int_0^{2\pi} \frac{d\varphi}{2\pi}\,\mathrm{e}^{\beta\cos(\varphi)} \tag{2}$$

without the usual error of $\mathrm{O}(N^{-2})$. It has machine precision instead for $N = 12$ or so. In this note we explain why this is so and estimate the in fact exponential convergence. All this is well-known to the experts, of course.

1.1 Euler Mac-Laurin

First we note

$$2T_N = h(f_0 + f_1 + \ldots + f_{2N-1}) \tag{3}$$

due to periodicity, $f_0 = f_{2N}$. Next we expand the (analytic) integrand

$$\int_u^{u+h} dx\, f(x) = \int_u^{u+h} dx \sum_{k=0}^{\infty} \frac{(x-u)^k}{k!} f^{(k)}(u) = \sum_{k=0}^{\infty} \frac{h^{k+1}}{(k+1)!} f^{(k)}(u) \tag{4}$$

and similarly

$$\int_u^{u+h} dx\, f(x) = \sum_{k=0}^{\infty} (-)^k \frac{h^{k+1}}{(k+1)!} f^{(k)}(u+h). \tag{5}$$

By symmetrizing over both variants we get

$$\int_u^{u+h} dx\, f(x) = \frac{1}{2}\sum_{k=0}^{\infty} \frac{h^{k+1}}{(k+1)!}[f^{(k)}(u) + (-)^k f^{(k)}(u+h)]. \tag{6}$$

1. The normalization $1/2\pi$ was not there before, but is nicer.

Adding this up for all subintervals

$$\int_0^{2\pi} dx\, f(x) - 2T_N(f) = h^2 \sum_{k=1}^{\infty} \frac{h^{2k-1}}{(2k+1)!} \sum_{n=0}^{2N-1} f^{(2k)}(x_n) \qquad (7)$$
$$= h^2 \sum_{k=1}^{\infty} \frac{h^{2k-2}}{(2k+1)!} 2T_N(f^{(2k)}),$$

all odd derivatives cancel and we have moved the zero'th order to the left hand side. This is essentially the Euler Mac-Laurin formula for estimating the difference between an integral and the approximating Riemann sum. In particular, the right hand side starts at order h^2.

For our peridioic function we may now iterate this as follows

$$\underbrace{\int_0^{2\pi} dx\, f''(x)}_{=0} - 2T_N(f'') = h^2 \sum_{k=1}^{\infty} \frac{h^{2k-2}}{(2k+1)!} 2T_N(f^{(2k+2)}) \qquad (8)$$

which puts the original error to $\mathrm{O}(h^4)$ with the integral vanishing by periodicity.

By iterating this process we may show that the error vanishes *faster than any power of* N^{-1}. In the second example we have integrated $\sin(x)$ from 0 to π and did find N^{-2} errors. If we want to replace this by an integral over a periodic function we have to take $|\sin(x)|$ which is *not analytic*!!!

1.2 Estimate of the convergence rate by a contour method

We rewrite I_0 as contour integral

$$I_0(\beta) = \oint \frac{dz}{2\pi i z} g(z), \quad g(z) = \mathrm{e}^{\beta(z+z^{-1})/2} = g(z^{-1}) \qquad (9)$$

which in the original form is around a unit circle but may be deformed (avoiding to cross the origin). Our approximation may be written

$$T_N = \frac{1}{N} \sum_{\{z_n\}} g(z_n), \quad z_n = \mathrm{e}^{2\pi i n/N}. \qquad (10)$$

Note that here N is comparable to $2N$ of the previous subsection.

To also write T_N as a contour integral we note first the identity

$$\prod_n (z - z_n) = z^N - 1. \qquad (11)$$

Both sides must coincide as they are polynomials of degree N with z_n as zeros and the highest power z^N with coefficient one. By differentiating the log we derive

$$\frac{1}{N} \sum_n \frac{1}{z - z_n} = \frac{z^{N-1}}{z^N - 1} \qquad (12)$$

This may be employed to write (10) as a contour integral with the help of the residue theorem

$$T_N = \left[\oint_{>} - \oint_{<} \right] \frac{dz}{2\pi i z} \frac{z^N}{z^N - 1} g(z) \tag{13}$$

with one integral along a circle with a radius larger than unity and with a smaller one such that effectively each pole at z_n is encircled in a positive sense and $g(z_n)$ is the residue. A transformation $z \to z^{-1}$ reflects the larger into the smaller circle yielding

$$T_N = \oint_{<} \frac{dz}{2\pi i z} \frac{1 + z^N}{1 - z^N} g(z) \tag{14}$$

and then

$$\Delta_N = T_N - I_0 = 2 \oint_{<} \frac{dz}{2\pi i z} \frac{z^N}{1 - z^N} g(z). \tag{15}$$

We want to compute this integral by a saddlepoint approximation and anticipate a saddle point of order $1/N$. To have a clear-cut power counting we change variables to $\alpha = zN$ and write

$$\Delta_N = 2N^{-N} \oint \frac{d\alpha}{2\pi i \alpha} \, \mathrm{e}^{NS(\alpha)} \tag{16}$$

with

$$S(\alpha) = \ln(\alpha) + (\beta/2)\alpha^{-1}. \tag{17}$$

where we have dropped terms that correspond to higher order $1/N$ corrections. The saddle point is at

$$\overline{\alpha} = \beta/2 \tag{18}$$

and setting (for real β) $\alpha = \overline{\alpha} + i\eta$ for the path of steepest descent thru $\overline{\alpha}$ we find

$$\Delta_N = \delta_N (1 + \mathrm{O}(N^{-1})) \tag{19}$$

with

$$\delta_N = 2N^{-N} \mathrm{e}^{NS(\overline{\alpha})} \frac{1}{\overline{\alpha}} \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} \, \mathrm{e}^{-\frac{1}{2} N S''(\overline{\alpha}) \eta^2} = \frac{2N^{-N}}{\overline{\alpha} \sqrt{2\pi N S''(\overline{\alpha})}} \, \mathrm{e}^{NS(\overline{\alpha})}. \tag{20}$$

Inserting numbers we find

$$\delta_N = \sqrt{\frac{2}{\pi N}} \left(\frac{2N}{\mathrm{e}\beta} \right)^{-N}. \tag{21}$$

In a brief test under `matlab` this gives an excellent description of the error. An impression is given in Figure 1. Note that for $N > 10$, the approximation is so excellent, that the deviation is covered by roundoff noise, i.a. T_N is practically at machine precision.

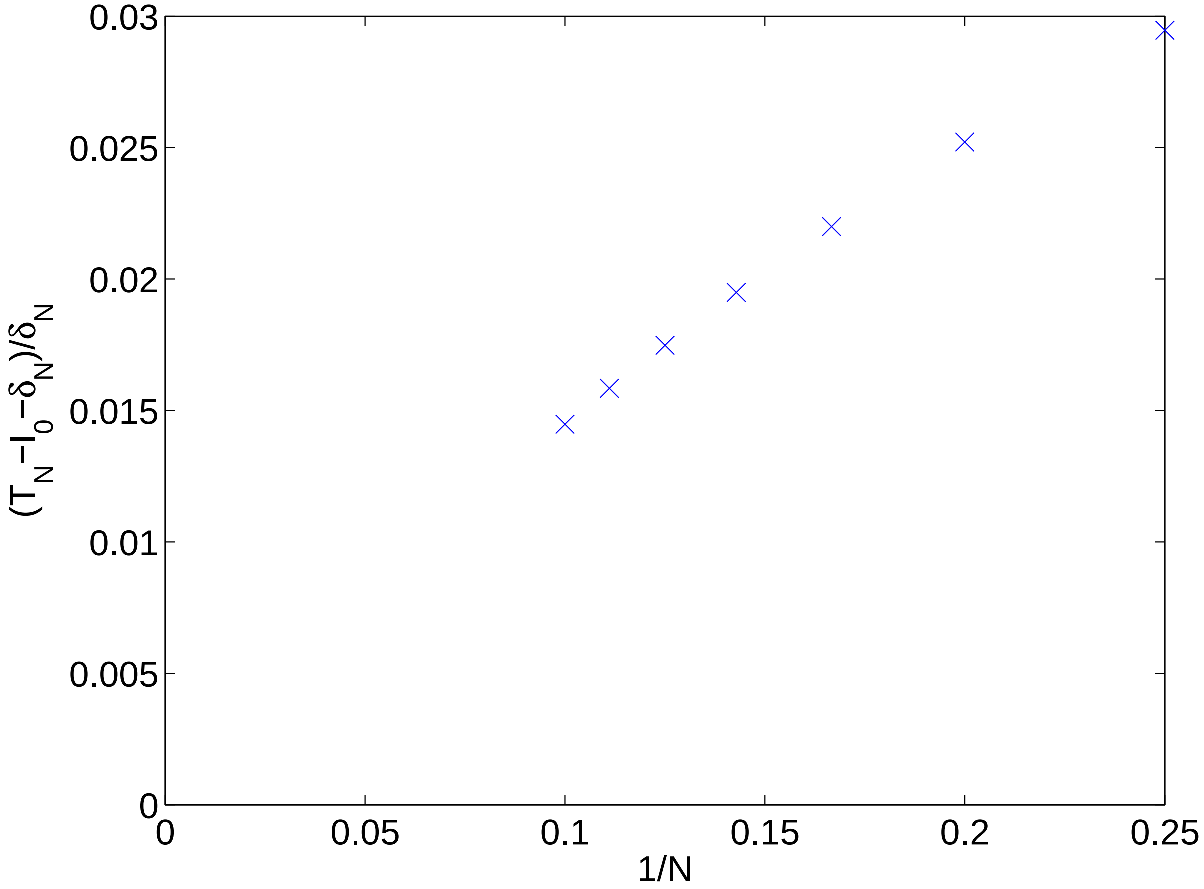

Figure 1. Relative error of Δ_N for $b = 1$ and $N = 4...10$.