Lecture 8

In lecture 7 we showed that for interpolation purposes, based on a polynomial approximant to the function to be interpolated, the precision with non-equispaced points is much higher than that with equi-spaced points. That conclusion, based on a particular example, is a general property, as is shown by Trefethen in his book. We also discussed the derivative matrices suitable to spectrally solve a differential equation, and concluded that loss of precision occurs when the derivative matrix (to be applied to the function whose derivatives we need to obtain) is based on a polynomial approximant. So, the conclusion here is that, rather than using approximants based on polynomials, approximants based on Fourier transforms (but needing to have equispaced points) are preferable. The reason is that the $\sin(kr)$ and $\cos(kr)$ have analytical derivatives $k\cos(kr)$ and $-k\sin(kr)$ that are bounded by the value of k, and not by the order of a poynomial. However, the support points for fourier expansions are uniformly spaced, and some of the accuracy is lost here. One of the purposes of the present lecture 8 is to review some of the properties of Fourier transforms, and present the associated derivative matrices, based on the book by Trefethen

We also tried out a simple S-IEM program that calculates the wave function for an exponential potential $V = \exp(-r/\alpha)$, with a wave number $k = 0.5$ inverse length, and $\alpha = 1$.

1 Fourier expansions

Based on Treferthen's Chapter 3.[3]

Given a continuous function $u(x)$ and the discrete set of meshpoints x_m $m = 1, 2, N$, then a function based on these meshpoints is $v(x)$, such that at the meshpoints

$$v_m = u(x_m) = v(x_m) \tag{1}$$

The Fourier transforms are

$$\begin{aligned} \hat{u}(k) &= \int_{-\infty}^{\infty} e^{-ikx} u(x) dx \\ \hat{v}(k) &= h \sum_{j=1}^{N} e^{-ik\ x_j} v_j,\ k = -\frac{N}{2} + 1, ... \frac{N}{2} \end{aligned} \tag{2}$$

The inverse transforms are

$$\begin{aligned} u(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \hat{u}(k) dk \\ v_j &= \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} e^{ik\ x_j} \hat{v}_k, \quad j = 1, ...N \end{aligned} \tag{3}$$

Theorem 1, Convergence of a Fourier Transform; From Trefethen p 30
a) If u has $p-1$ continuous derivatives in $L^2(\mathbb{R})$, and a p'th derivative of bounded

value, then

$$\hat{u}(k) = O(|k|^{-p-1}) \text{ as } k \to \infty \tag{4}$$

b) If u has ∞ many continuous derivatives in $L^2(\mathbb{R})$, then

$$\hat{u}(k) = O(|k|^{-m}) \text{ as } k \to \infty \tag{5}$$

for every $m > 0$. The latter means that the convergence is super algebraic.

Example 1

$$u(x) = \pi e^{-\sigma|x|}$$
$$\hat{u}(k) = \frac{\sigma}{k^2 + \sigma^2},$$

Here $\hat{u}(k)$ decays algebraically because $p = 1$ (note the absolute value in the exponent)

Example 2

$$u(x) = e^{-x^2/2\sigma^2}$$
$$\hat{u}(k) = \sigma\sqrt{\pi/2}\ e^{-\sigma^2 k^2/2}$$

The Fourier transform decays superalgebraically because u has an infinite number of derivatives.

Theorem 3, Convergence of a discrete Fourier transform; From Trefethen p 30

Let $u \in L^2(\mathbb{R})$, and let v be the grid function defined on $h\mathbb{Z}$ by $v_j = u(x_j)$. (Note that $h\mathbb{Z}$ has an infinite number of discrete points separated by the distance h, going from $-\infty$ to $+\infty$.) Then for all $k \in [-\pi/h, \pi/h]$

a) If u has $p-1$ continuous derivatives in $L^2(\mathbb{R})$, and a p'th derivative of bounded value, $(p \geq 1)$ then

$$|\hat{v}(k) - \hat{u}(k)| = O(h^{p+1}) \text{ as } h \to 0 \tag{6}$$

b) If u has ∞ many continuous derivatives in $L^2(\mathbb{R})$, then

$$|\hat{v}(k) - \hat{u}(k)| \ = O(h^m) \text{ as } h \to 0 \text{ for every } m > 0 \tag{7}$$

Theorem 4 Accuracy of a Fourier spectral differentiation, From Trefethen p 34

Let $u \in L^2(\mathbb{R})$ have a v'th derivative $(v \geq 1)$ of bounded variation, and let w be the v'th spectral derivative of u on the grid $h\mathbb{Z}$. Then, for all $x \in h\mathbb{Z}$ the following holds uniformly:

a) If u has $p-1$ continuous derivatives in $L^2(\mathbb{R})$ for some $p \geq v+1$, and a p'th derivative of bounded value, $(p \geq 1)$ then

$$|w_j - u^{(v)}(x_j)| = O(h^{p-v}) \text{ as } h \to 0 \tag{8}$$

b) If u has ∞ many continuous derivatives in $L^2(\mathbb{R})$, then

$$|w_j - u^{(v)}(x_j)| \ = O(h^m) \text{ as } h \to 0 \text{ for every } m > 0 \tag{9}$$

(i.e., the convergence is super-algebraic).

2 Fourier spectral differentiation on bounded periodic grids.

For periodic functions whose discrete support points are defined on a finite, evenly spaced, grid $x_1 = h,\ x_2 = 2h,\ x_{N/2} = \pi..x_N = 2\pi$, where $h = 2\pi/N$, and N is even, the Fourier transforms are given by

$$\hat{v}_k = h\sum_{j=1}^{N} e^{-ikx_j} v_j,\ \ k = -\frac{N}{2}+1, ..., \frac{N}{2} \tag{10}$$

and the function based on these meshpoints is $v(x)$, such that at the meshpoints according to Eq. (1) $v_m = u(x_m) = v(x_m)$, the inverse Fourier transform is

$$v_j = \frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}'' \ e^{-ikx_j}\ \hat{v}_k\ ,\ j = 1, 2, .., N \tag{11}$$

where the " means that the terms with $k = \pm N/2$ are multiplied by 1/2, and the periodicity property sets $\hat{v}_{-N/2} = \hat{v}_{N/2}$. The corresponding band-limited interpolant is

$$p(x) = \frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}'' \ e^{-ikx}\ \hat{v}_k\ ,\ x \in [0, 2\pi]. \tag{12}$$

Bsed on these results, the band limited interpolant to a delta function $\delta(x)$ is the *periodic sinc function* S_N

$$S_N(x) = \frac{\sin(\pi x/h)}{(2\pi/h)\ \tan(x/2)} \tag{13}$$

given by Eq. (3.7) of Trefethen. This function is equal to 1 at points $x = 0$ and 2π, and vanishes at all intermediate discrete points $x_n = nh$, $n = 1, 2, ..N-1$. This function is the equivalent of a Lagrange polynomial, and can be used to build up an interpolant to the function v

$$p(x) = \sum_{m=1}^{N} v_m S_N(x - x_m). \tag{14}$$

This is the basic result for Fourier-transforms of periodic functions. The derivatives dp/dx at the support points x_m can be obtained analytically in terms of the derivatives of the functions $S_N(x - x_m)$. If $y = (x - x_m)$ one finds

$$S'_N(y) = \frac{dS_N(y)}{dy} = \frac{1}{2}\frac{\cos(\pi y/h)}{\tan(y/2)} - \frac{\sin(\pi y/h)}{(4\pi/h)\sin^2(y/2)}. \tag{15}$$

From the above result one finds that

$$S'_N(-y) = -S'_N(y) \tag{16}$$

and that

$$S'_N(x_n - x_m) = \frac{\cos[\pi(n-m)]}{2\tan[(n-m)\pi/N]}. \tag{17}$$

If $n-m$ is denoted as j, the final result, in agreement with Eq. (3.9) of Trefethen, is

$$S'_N = \frac{(-)^j}{2\tan(j\pi/N)},\ j = n-m. \tag{18}$$

According to the derivative of Eq. (14) the first order derivative matrix is given by

$$D_N = \begin{pmatrix} 0 & \frac{1}{2}\cot(\frac{1h}{2}) & -\frac{1}{2}\cot(\frac{2h}{2}) & \frac{1}{2}\cot(\frac{3h}{2}) & \cdots & \frac{1}{2}\cot(\frac{(N-1)h}{2}) \\ -\frac{1}{2}\cot(\frac{1h}{2}) & 0 & \frac{1}{2}\cot(\frac{1h}{2}) & -\frac{1}{2}\cot(\frac{2h}{2}) & \cdots & -\frac{1}{2}\cot(\frac{(N-2)h}{2}) \\ \frac{1}{2}\cot(\frac{2h}{2}) & -\frac{1}{2}\cot(\frac{1h}{2}) & 0 & \frac{1}{2}\cot(\frac{1h}{2}) & \cdots & \frac{1}{2}\cot(\frac{(N-3)h}{2}) \\ -\frac{1}{2}\cot(\frac{3h}{2}) & \frac{1}{2}\cot(\frac{2h}{2}) & -\frac{1}{2}\cot(\frac{1h}{2}) & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & & \ddots & \frac{1}{2}\cot(\frac{1h}{2}) \\ -\frac{1}{2}\cot(\frac{(N-1)h}{2}) & \frac{1}{2}\cot(\frac{(N-2)h}{2}) & -\frac{1}{2}\cot(\frac{(N-3)h}{2}) & \cdots & -\frac{1}{2}\cot(\frac{1h}{2}) & 0 \end{pmatrix} \tag{19}$$

Trefethen gives an example for the differentiation of the function $\exp[\sin(x)]$ for x in the interval $[0, 2\pi]$, with $N = 24$. The accuracy of the derivative of this periodic function is excellent, of the order of 10^{-12}, while the accuracy of the derivative of a "hat" function is very poor.

Trefethen also gives the elements of the second order derivative of a periodic function, with the result $S''_N(x_j) = -\pi^2/(3h^2) - 1/6$ for $j = 0$ $(Mod\ N)$, and $S''_N(x_j) = -(-1)^j/[2\sin^2(jh/2)]$ for $j \neq 0$ $(Mod\ N)$. For small values of h, these matrix elements for small values of j are of the order of h^{-2}, which is still smaller than the values of order h^{-4} found for the second order derivative matrices based on orthogonal polynomials.

3 Convergence of a polynomial approximation to a function

Based on Ref. **[4]**

Since the expansions into a set of polynomials amounts to creating a polynomial $P_N(x)$ of order N which, for a given set of meshpoints $\xi_i,\ i = 1, 2, ...N$ has values that are equal to the function being expanded, i.e., $P_N(\xi_i) = f(\xi_i)$, $i = 1, 2, ...N$, it is of interest to know how well P_N approaches f at points x other than the meshpoints. That knowledge determines the interpolation error. Two theorems are relevant. The second theorem shows that the Chebyshev meshpoints give rise to the best interpolation.

Theorem 1. (Cauchy iterpolation error theorem)

Let $f(x)$ be a function sufficiently smooth so that it has at least $N+1$ continuous derivatives on the interval $[-1, 1]$, and let P_N be its Lagangian interpolant of degree N for $x \in [-1,1]$, the upper bound of the interpolation error is given by

$$f(x) - P_N(x) \leq \frac{1}{(N+1)!} f^{(N+1)}(\bar{x}) \prod_{i=1}^{N} (x - \xi_i) \tag{20}$$

for some $\bar{x} \in [-1,1]$.

Deloff notices that in order to minimize the interpolation error $f(x) - P_N(x)$ for any function f the product term in Eq. (10) should be minimized. This product term has the monic character, i.e., the coefficient of the highest power of x is unity. The theorem below states that the best choice of the ξ_i are the Chebyshev support points.

Theorem 2. (Chebyshev minimal amplitude theorem) Out of all monic polynomials of degree N, the unique polynomial which has the smallest maximum on $[-1,1]$ is the Chebyshev polynomial T_N divided by 2^{N-1}, i.e., all monic polynomials $Q_N(x)$ satisfy he inequality

$$\max |Q_N(x)| \geq \max |T_N(x)/2^{N-1}| = 1/2^{N-1} \tag{21}$$

for all $x \in [-1,1]$.

Comments: The polynomial P_N can be obtained either by a sum over Lagrange functions times coefficients, or a sum over Chebyshev (or other orthogonal) polynomials, so that the maximum power of x is N. Hence, according to Theorem 1, for a given N, the error $f(x) - P_N(x)$ is less lor equal to a constant factor times the monic polynomial $\prod_{i=1}^{N}(x - \xi_i)$. According to Theorem 2 the monic polynomial that has the minimum amplitude is $T_N(x)$, if the $\{\xi_i\}_N$ are the zeros of T_{N+1}. Further, according to Trefethen, Chapter 5, these amplitudes are all uniform in x, i.e., they are all bounded by the same superating constant. This is not the case for equispaced points which are used in the construction of the interpolant $P_N(x)$, as illustrated in Chapter 5, Output 9, and reproduced in the section below.

The rule of thumb for expansions into Chebyshev Polynomials is that the truncation error in the expansion after N terms is closely given by the magnitude of the next coefficient of the expansion, a_{N+1}. An example was given in Fig. **??** in Lecture 6 for the expansion of $\exp(x)$ in the interval $[-1,1]$. The figure showed that the error ϵ_n divided by a_n of the expansion $\exp(x) = \sum_{k=1}^{n} a_k T_{k-1}(x) + \epsilon_n$ truncated at n was in magnitude ≤ 1, and was uniform in x.

For functions that are periodic, a Fourier expansion may converge faster than a Chebyshev expansion. A numerical example given below is the expansion of a Gaussian function

$$f(r) = \exp(-r^2), \quad 0 \leq r \leq 6.$$

The Fourier expansion is based on the result $\int_0^\infty \exp(-x^2)\cos(b_n x)dx = [sqrt(\pi)/2]\exp(-0.25 b_n^2)$, with $b_n = (\pi/12)(2n+1)$, and $n = 0,1,2,..$ so chosen that $\cos(b_n 6) = 0$. The Chebyshev expansion is performed with 21 Chebyshev functions, using a mesh grid as the zeros of the Chebyshev polynomial $T_{21}(x)$ in the interval $[-1,1]$. The upper limit 6 of the radial interval is chosen large enough such that

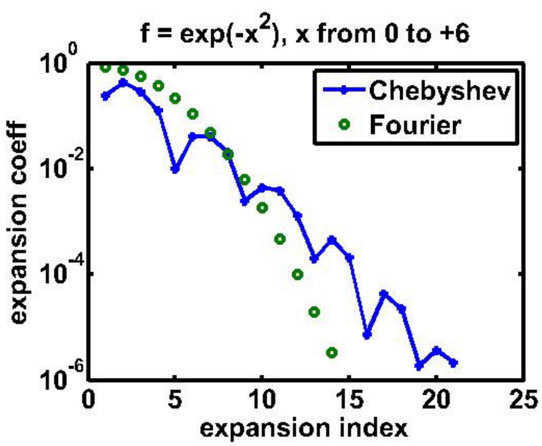

Figure 1: Comparison of the Fourier and Chebyshev expansion coefficients for $f(r) = \exp(-r^2)$, $0 \leq r \leq 6$. The text descibes the discretization of either expansion.

$\exp(-6^2) = 2.3 \times 10^{-16}$ is smaller than the numerical accuracy of MATLAB. The comparison of the two expansions is illustrated in Fig. 1. It shows that in this case the Fourier expasion converges significantly faster.

References

[1] Gonzales, R.A., Eisert, J., Koltracht, I., M. Neumann, M. and G. Rawitscher, G., "Integral Equation Method for the Continuous Spectrum Radial Schrödinger Equation", *J. of Comput. Phys.*, 1997, **134**, 134-149;

[2] J. Power and G. Rawitscher, Phys. Rev. E 86 (2012) 066707.

[3] L. N. Trefethen, *Spectral Methods in MATLAB*, (SIAM, Philadelphia, PA, 2000);

[4] A. Deloff, Ann. Phys. (NY) **322** (2007) 1373–1419.