Fourier interpolation / differentiation

We have considered polynomial interpolation as a means to produce numerical derivatives. We shall continue with this plan soon, using Chebyshev, or more generally Jacobi polynomial interpolants.

Before going in that direction, however, we consider an alternative: Fourier expansion!

How would we compute a Fourier approximation (interpolant) for a function given only on an equispaced mesh?

Ans: we rely on Fourier-coefficient integral formula together with the trapezoidal rule!

Benefits:

1) Straightforward evaluation of the interpolant coefficients

2) Very fast convergence for smooth and periodic functions. (See e.g. problem 1, Set II.)

Disadvantages:

1) Restricted to periodic functions.

We will remove the restrictions later. For now we consider periodic problems.

Fourier Coefficients

Let u denote a smooth 2π-periodic function.

The coefficients $\hat{u}_k$ in the Fourier expansion

$$u(x) = \sum_{k=-\infty}^{\infty} \hat{u}_k \, e^{ikx}$$

are given by

$$\hat{u}_k = \frac{1}{2\pi} \int_0^{2\pi} u(x) \, e^{-ikx}$$

Idea: use the trapezoidal rule, which, gives excellent convergence for smooth and periodic functions (cf. problem sets I and II, additional discussion below). Equispaced points!

In any case: what do we obtain when we approximate $\hat{u}_k$ by means of the trapezoidal rule?

It suffices to see what results as the trapezoidal rule is applied to e^{ikx}!

The result is (using N points $x_j = \frac{2\pi}{N} j$):

$$\frac{2\pi}{N} \sum_{j=0}^{N-1} e^{\frac{2\pi i k}{N} j} =$$

$$= \frac{2\pi}{N} \sum_{j=0}^{N-1} \left[e^{\frac{2\pi i k}{N}} \right]^j =$$

$$= \frac{2\pi}{N} \frac{\left[e^{\frac{2\pi i k}{N}} \right]^N - 1}{e^{\frac{2\pi i k}{N}} - 1} =$$

$$= 2\pi \cdot \begin{cases} 0 & \text{if } \overbrace{k \text{ is not a multiple of } N}^{k \not\equiv 0\,(N)} \\ 1 & \text{if } k \text{ is } \underbrace{\text{a multiple of } N}_{k \equiv 0\,(N)}. \end{cases}$$

Thus, the trapezoidal approximation for the integral of u equals

$$2\pi \sum_{\substack{k=-\infty \\ k \equiv 0\ (N)}}^{\infty} \hat{u}_k =$$

$$= 2\pi \cdot \left(\ldots \hat{u}_{-2N} + \hat{u}_{-N} + \hat{u}_0 + \hat{u}_N + \hat{u}_{2N} \ldots \right)$$

(The exact integral equals $2\pi \hat{u}_0$!)

Discrete Fourier Expansions

In the previous class we showed that the trapezoidal approximation, using the N points $x_j = \frac{2\pi}{N} j$, $(0 \le j \le N-1)$, for the integral of a 2π-periodic function

$$u(x) = \sum_{k=-\infty}^{\infty} \hat{u}_k e^{ikx}$$

equals

$$2\pi \sum_{\substack{k=-\infty \\ k \equiv 0 \, (N)}}^{\infty} \hat{u}_k =$$

$$= 2\pi \cdot \left(\dots \hat{u}_{-2N} + \hat{u}_{-N} + \hat{u}_0 + \hat{u}_N + \hat{u}_{2N} \dots \right).$$

(The exact integral equals $2\pi \cdot \hat{u}_0$.)

(Note that, in particular, for a function

$$v \in \operatorname{span}\left\{ e^{ikx} \right\}_{0 \le |k| \le N-1} \quad \text{we have}$$

the exact relation

$$\frac{1}{2\pi}\int_0^{2\pi} v(x)\,dx = \frac{1}{N}\sum_{j=0}^{N-1} v(x_j).$$

We thus define the trapezoidal approximation

$$\tilde{u}_k = \frac{1}{N}\sum_{j=0}^{N-1} u(x_j)\, e^{-ikx_j} \qquad (k=0, \pm 1, \pm 2, \dots)$$

for the Fourier coefficients $\hat{u}_k$.

Note that the approximate coefficients $\tilde{u}_k$ are N-periodic:

$$\tilde{u}_{k\pm N} = \frac{1}{N}\sum_{j=0}^{N-1} u(x_j)\, e^{-i(k\pm N)x_j} =$$

$$= \frac{1}{N}\sum_{j=0}^{N-1} u(x_j)\, e^{-ikx_j}\underbrace{e^{\mp 2\pi i j}}_{=1} = \tilde{u}_k$$

In view of type of manipulations we are considering we define

$$\langle u, v\rangle_N = \frac{1}{N}\sum_{j=0}^{N-1} u(x_j)\,\overline{v(x_j)}$$

The trapezoidal rule expression on page 183 tells us that, letting

$$E_l(x) = e^{ilx} \quad (l \in \mathbb{Z})$$

and $N \geq 1$, for $k, m \in \mathbb{Z}$ we have

$$\langle E_k, E_m\rangle = \begin{cases} 1 & \text{if } k-m = lN \ (l\in\mathbb{Z}) \\ 0 & \text{otherwise} \end{cases}$$

This a discrete analog of the orthonormality relation

$$(E_k, E_m) = \frac{1}{2\pi}\int_0^{2\pi} e^{i(k-m)x}\,dx = \delta_{km}.$$

In view of the periodicity of Fourier coefficients

we have

$$\tilde{u}_{-N/2} = \tilde{u}_{N/2} \qquad (N \text{ even}).$$

These two modes are said to be "aliased".

For simplicity we restrict treatment to even

values of N, and we consider the set of modes

$$E_k \text{ with } -\frac{N}{2} \leq k \leq \frac{N}{2}.$$

In view of periodicity, in our treatment the

coefficients are modified so that both the $-N/2$ and

$N/2$ coefficients are present, with half weight each;
the discrete Fourier coefficients are thus re-defined according to

(1) $$\tilde{u}_k = \frac{1}{N c_k} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j} \qquad (-N/2 \le k \le N/2)$$

where
$$c_k = \begin{cases} 1 & \text{for } |k| < N/2 \\ 2 & \text{for } k = \pm N/2 . \end{cases}$$

(Other alternatives are also often used in practice, such as assigning the full weight to $\tilde{u}_{-N/2}$ and setting $\tilde{u}_{N/2} = 0$.)

This is the (forward) discrete Fourier transform of $u(x)$ associated with the discretization
$$\left\{ x_j = \frac{2\pi}{N} j : \; j = 0, \ldots, N-1 \right\}$$

Note that, by periodicity, we have only N independent discrete coefficients.

<u>Fact</u>: the discrete Fourier expansion is interpolatory.

In other words, defining $I_N(u)$ by

$$\Big(I_N(u)\Big)(x) = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \tilde{u}_k\, e^{ikx},$$

given by (1)

for any given function u defined in $[0,2\pi]$

we have

$$\Big(I_N(u)\Big)(x_\ell) = u(x_\ell) \qquad (2)$$

for $0 \leqslant \ell \leqslant N-1$.

<u>Proof</u>: we have

$$\left(I_N(u)\right)(x) = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \left(\frac{1}{N c_k} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j} \right) e^{ikx} =$$

$$\sum_{j=0}^{N-1} \underbrace{\left[\frac{1}{N} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \frac{1}{c_k} e^{ik(x-x_j)} \right]}_{h_j(x)} u(x_j) \qquad (3)$$

But, using p. 181 we have

$$h_j(x_\ell) = \frac{1}{N} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \frac{1}{c_k} e^{ik(x_\ell - x_j)} =$$

$$= \frac{1}{N} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \frac{1}{c_k} e^{ik\frac{2\pi}{N}(\ell - j)} =$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} e^{ik\frac{2\pi}{N}(\ell - j)} = \begin{cases} 0 & \ell - j \not\equiv 0 \ (N) \\ 1 & \ell - j \equiv 0 \ (N), \end{cases}$$

and, thus, equation (2) follows.

Fact: we have

$$h_j(x) = \frac{1}{N} \sin\left[N \frac{x - x_j}{2}\right] \cot\left[\frac{x - x_j}{2}\right] \quad (4)$$

(proof omitted; similar to Dirichlet kernel derivation; see p. 27 STW.)

Equations (3) and (4) provide the analog

$$\left(I_N(u)\right)(x) = \sum_{j=0}^{N-1} h_j(x)\, u(x_j) \quad (5)$$

of the Lagrange interpolation formula in the context of discrete Fourier interpolation.

Differentiation of equation (5) can be used as a basis for a PDE solver, even for large values of N.

<u>Note</u>: use of (5) to obtain derivatives at all N points $x_0, \dots, x_{N-1}$ requires $\mathcal{O}(N^2)$ cost as N grows.

<u>Note</u>: The relations (1) and (2), which we rewrite here as

$$\tilde{u}_k = \frac{1}{N c_k} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j}$$

$$u(x_\ell) = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \tilde{u}_k e^{ikx_\ell}$$

are the discrete analogs of the direct and inverse Fourier transform.

Alternative to $\mathcal{O}(N^2)$ algorithm:

the Fast Fourier Transform (FFT)

(Cooley - Tuckey 1965, Gauss ~ 1806)

The calculation of the discrete Fourier transform

$$F_k = \sum_{j=0}^{N-1} e^{2\pi i jk/N} f_j$$

can be reduced as follows:

$$F_k = \sum_{j=0}^{N/2-1} e^{2\pi i k(2j)/N} f_{2j} + \sum_{j=0}^{N/2-1} e^{2\pi i k(2j+1)/N} f_{2j+1}$$

or, letting $W \equiv e^{2\pi i/N}$

$$F_k = \sum_{j=0}^{N/2-1} e^{2\pi i kj/(N/2)} f_{2j} + W^k \sum_{j=0}^{N/2-1} e^{2\pi i kj/(N/2)} f_{2j+1}$$

or,

$$F_k = F_k^e + W^k F_k^o$$

Thus we have reduced the problem to evaluation of two transforms of size $N/2$.

Direct evaluation of these requires

$$2\left(\frac{N}{2}\right)^2 = \frac{N^2}{2} \quad \text{operations.}$$

Cheaper! And we can repeat!

We eventually get to

$$F_k^{eoeeoeo\cdots oee} = f_n \qquad \text{for some } n$$

and we are done. If $N = 2^p$, then a total of $p = \log_2 N$ steps suffice.

At N operations per step, a total cost of $N \log_2(N)$ results.

How about N not equal to a power of 2?

This is also Ok, works well as long as N does not contain large prime factors.

(One can always use a discretization with an adequate value of N, equal to products of powers of small primes.)

Matlab format

$$\left\{ v(j) = u(x_{j-1}) \right\}_{j=1}^{N}, \quad x_j = \frac{2\pi j}{N}$$

$\tilde{v} = \text{fft}(v)$ returns $\left\{ \tilde{v}_k \right\}_{k=1}^{N}$ where

$$\tilde{v}(k) = \sum_{j=1}^{N} v(j)\, e^{-2\pi i (j-1)(k-1)/N}$$

The inverse FFT is given by

$$v = \text{ifft}(\tilde{v})$$

returns the physical values

$$\left\{ v(j) \right\}_{j=1}^{N} \quad \text{given by}$$

$$v(j) = \frac{1}{N} \sum_{k=1}^{N} \tilde{v}(k)\, e^{2\pi i (j-1)(k-1)/N}$$

It is important to keep in mind the following relationships:

$$u(x_j) = v(j+1), \quad x_j = \frac{2\pi j}{N}, \quad 0 \le j \le N-1$$

$$\tilde{u}_k = \frac{1}{N} \tilde{v}(k+1) \qquad 0 \le k \le \frac{N}{2} - 1$$

$$\tilde{u}_k = \frac{1}{N} \tilde{v}(k+N+1) \qquad -\frac{N}{2} + 1 \le k \le -1$$

$$\tilde{u}_{-N/2} = \tilde{u}_{N/2} = \frac{1}{2N} \tilde{v}\left(\frac{N}{2} + 1\right)$$

$$\underbrace{u(x_0)}_{v(1)}, \quad \dots, \quad \underbrace{u(x_{N-1})}_{v(N)}$$

$$\tilde{u}_0, \dots, \tilde{u}_{\frac{N}{2}-1}, \; 2\tilde{u}_{\frac{N}{2}}, \qquad \tilde{u}_{-\frac{N}{2}+1}, \dots, \tilde{u}_{-1}$$

$$\frac{\tilde{v}(1)}{N}, \quad \frac{\tilde{v}(N/2)}{N}, \quad \frac{\tilde{v}(\frac{N}{2}+1)}{N}, \qquad \frac{\tilde{v}(N/2+2)}{N} \qquad , \frac{\tilde{v}(N)}{N}$$

Discrete Fourier approach: high-order approximation, convergence, fast (FFT).

Limitation: Periodicity requirement

IDEA!

Given a smooth function

$$f : [-1,1] \to \mathbb{R}$$

consider $f(\cos(\theta))$: periodic function of θ

Fourier series (cosine series)

$$f(\cos(\theta)) = \sum_{k=0}^{\infty} a_k \cos(k\theta)$$

where

$$a_k = \frac{2}{\pi c_k} \int_0^{\pi} f(\cos(\theta)) \cos(k\theta)\, d\theta$$

$$(c_0 = 2, \; c_k = 1 \text{ for } k > 0)$$

$$x = \cos(\theta)$$

$$\theta = \arccos(x)$$

$$f(x) = \sum_{k=0}^{\infty} a_k \underbrace{\cos(k \arccos(x))}_{\text{polynomial}}$$

Chebyshev approximation

Given a smooth function

$$f : [-1,1] \longrightarrow \mathbb{R}$$

consider $f(\cos(\theta))$: 2π-periodic function of θ.

This is also an even function of θ, and thus

1) All of its sine coefficients vanish:

$$f(\cos(\theta)) = \sum_{k=0}^{\infty} a_k \cos(k\theta); \quad \text{and}$$

2) Its Fourier coefficients a_k can be obtained as integrals between 0 and π: letting $c_0 = 2$ and $c_k = 1$ for $k > 0$,

we have

$$a_k = \frac{1}{\pi c_k} \int_{-\pi}^{\pi} \underbrace{f(\cos(\theta))\cos(k\theta)}_{\text{even}} d\theta ,$$

and, thus

$$a_k = \frac{2}{\pi c_k} \int_0^{\pi} f(\cos(\theta)) \cos(k\theta)\, d\theta. \qquad (1)$$

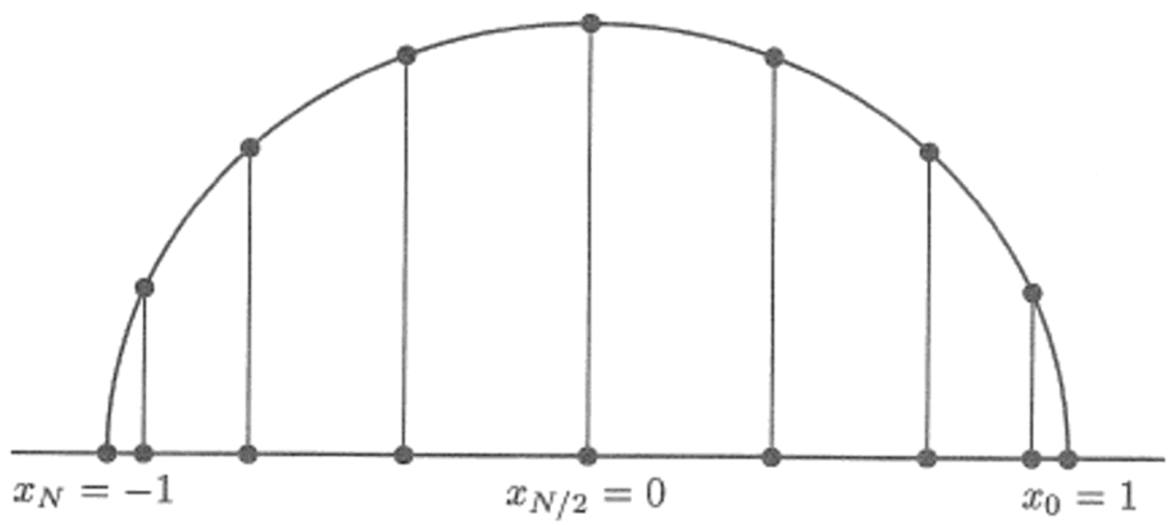
The discrete Fourier expansion methods can be used to obtain approximate versions of the coefficients a_k using the trapezoidal rule on the complete 2π periodcity interval $[-\pi, \pi]$ (in the variable θ), and using equispaced discretization points in the variable θ. But since

$$f(\cos(\theta)) \cos(k\theta)$$

is an even function, the sum is reduced, as in (1), to twice a sum over discretization points θ_j in the interval $[0, \pi]$.

Of course, this requires use of the function values $f(\cos(\theta_j))$ of the function f at points

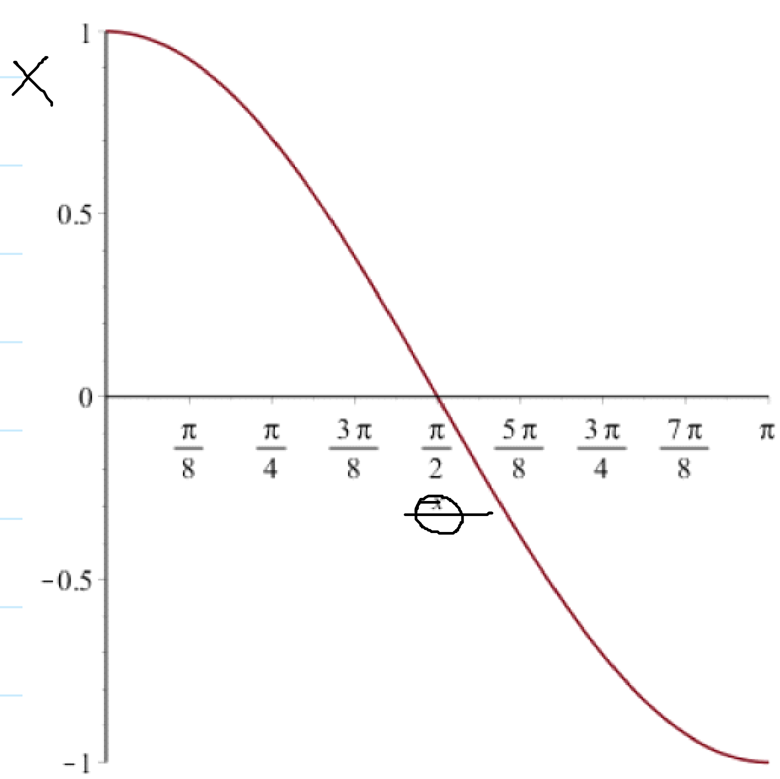
$$x_j = \cos(\theta_j)$$



The Chebyshev points x_j are the projections onto the x-axis of equally spaced points on the unit circle

Several different choices can be made for the equispaced points θ_j, including both endpoints, only one endpoint, or neither endpoint (the latter using $\theta_1 = h/2$, $\theta_2 = \frac{3h}{2}$, $\theta_3 = \frac{5}{2}h$, $\ldots$, $\theta_n = \pi - \frac{h}{2}$

The change of variables $x = \cos(\theta)$ inverts the directions: x goes from 1 to -1 as θ goes from 0 to π.



This graph also shows how equispaced points θ_j are transformed into points $x_j = \cos(\theta_j)$ which accumulate toward the endpoints $x = \pm 1$ of the x interval.

The cosine expansions of the form

$$f(\cos(\theta)) = \sum_k a_k \cos(k\theta)$$

containing either finitely-many or infinitely-many terms (as may arise from e.g. a discrete or a continuous transform, respectively) can be re-expressed in the x variable:

$$f(x) = \sum_k a_k \cos(k \arccos(x)).$$

Let us call

$$T_k(x) = \cos(k \arccos(x)).$$

We show that $T_k(x)$ is a polynomial of degree k.

(Chebyshev is sometimes spelled Tchebyshev, which explains the use of the T_k notation.)

To do this we first note the trigonometric relation

$$\cos((k+1)\theta) + \cos((k-1)\theta) = 2\cos(\theta)\cos(k\theta)$$

which tells us that

$$T_{k+1}(x) + T_{k-1}(x) = 2x\,T_k(x) \qquad (2)$$

This is a "three-term recurrence relation".

Given that, clearly

$$T_0(x) = 1 \quad \text{and} \quad T_1(x) = x$$

it follows inductively that $T_k(x)$ is a polynomial of degree k for all non-negative integers k, as claimed.

Note also that, importantly, the relation (2) enables recursive evaluation of <u>all</u> $T_k(x)$

at any given $x \in \mathbb{R}$ without recourse to (expensive) evaluation of the cos and arccos functions.

Chebyshev Expansion

Using the Chebyshev polynomials $T_k(x)$ we re-express the expansion

$$f(\cos(\theta)) = \sum_{k=0}^{\infty} a_k \cos(k\theta)$$

in the "Chebyshev expansion" form

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x)$$

Converges <u>fast</u> for arbitrary, non-periodic (smooth) functions. We will exploit such expansions for computational purposes.