# Chapter 7

# Spectral Interpolation, Differentiation, Quadrature

## 7.1 Interpolation

### 7.1.1 Bandlimited interpolation

While equispaced points generally cause problems for polynomial interpolation, as we just saw, they are the natural choice for discretizing the Fourier transform. For data on $x_j = jh$, $j \in \mathbb{Z}$, recall that the semidiscrete Fourier transform (SFT) and its inverse (ISFT) read

$$\hat{f}(k) = h \sum_{j \in \mathbb{Z}} e^{-ikx_j} f_j, \qquad f_j = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{ikx_j} \hat{f}(k)\, dk.$$

The idea of spectral interpolation, or bandlimited interpolation, is to evaluate the ISFT formula above at some point $x$ not equal to one of the $x_j$.

**Definition 21.** *(Fourier/spectral/bandlimited interpolation on $\mathbb{R}$) Let $x_j = jh$, $j \in \mathbb{Z}$. Consider $f : \mathbb{R} \mapsto \mathbb{R}$, its restriction $f_j = f(x_j)$, and the SFT $\hat{f}(k)$ of the samples $f_j$. Then the spectral interpolant is*

$$p(x) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{ikx} \hat{f}(k)\, dk.$$

We can view the formula for $p(x)$ as the inverse Fourier transform of the compactly supported function equal to $\hat{f}(k)$ for $k \in [-\pi/h, \pi/h]$, and zero otherwise. When the Fourier transform of a function is compactly supported, we say that that function is *bandlimited*, hence the name of the interpolation scheme.

**Example 22.** *Let*

$$f_j = \delta_{0j} = \begin{cases} 1 & \text{if } j = 0; \\ 0 & \text{if } j \neq 0. \end{cases}$$

*Then the SFT is* $\hat{f}(k) = h$ *for* $k \in [-\pi/h, \pi/h]$ *as we saw previously. Extend it to* $k \in \mathbb{R}$ *by zero outside of* $[-\pi/h, \pi/h]$. *Then*

$$p(x) = \frac{\sin(\pi x/h)}{\pi x/h} = sinc(\pi x/h).$$

*This function is also called the Dirichlet kernel. It vanishes at* $x_j = jh$ *for* $j \neq 0$, *integer.*

**Example 23.** *In full generality, consider now the sequence*

$$f_j = \sum_{k \in \mathbb{Z}} \delta_{jk} f_k.$$

*By linearity of the integral,*

$$p(x) = \sum_{k \in \mathbb{Z}} f_k sinc(\pi(x - x_k)/h).$$

*The interpolant is a superposition of sinc functions, with the samples* $f_j$ *as weights. Here sinc is the analogue of the Lagrange elementary polynomials of a previous section, and is called the* interpolation kernel. *For this reason, bandlimited interpolation sometimes goes by the name Fourier-sinc interpolation.*

*(Figure here for the interpolation of a discrete step.)*

In the example above we interpolate a discontinuous function, and the result is visually not very good. It suffers from the same Gibbs effect that we encountered earlier. The smoother the underlying $f(x)$ which $f_j$ are the samples of, however, the more accurate bandlimited interpolation.

In order to study the approximation error of bandlimited interpolation, we need to return to the link between SFT and FT. The relationship between $p(x)$ and $f_j$ is *sampling*, whereas the relationship between the FT

$\hat{f}(k)\chi_{[-\pi/h,\pi/h](k)}$ and the SFT $\hat{f}(k)$ is *periodization*. We have already alluded to this correspondence earlier, and it is time to formulate it more precisely.

(Figure here; sampling and periodization)

**Theorem 14.** *(Poisson summation formula, FT version) Let* $u : \mathbb{R} \mapsto \mathbb{R}$*, sufficiently smooth and decaying sufficiently fast at infinity. (We are deliberately imprecise!) Let* $v_j = u(x_j)$ *for* $x_j = jh$*,* $j \in \mathbb{Z}$*, and*

$$\hat{u}(k) = \int_{\mathbb{R}} e^{-ikx} u(x)\, dx, \qquad (FT), \qquad k \in \mathbb{R},$$

$$\hat{v}(k) = h \sum_{j\in\mathbb{Z}} e^{-ikx_j} u(x_j). \qquad (SFT), \qquad k \in [-\pi/h, \pi/h].$$

*Then*

$$\hat{v}(k) = \sum_{m\in\mathbb{Z}} \hat{u}(k + m\frac{2\pi}{h}), \qquad k \in [-\pi/h, \pi/h] \tag{7.1}$$

In some texts the Poisson summation formula is written as the special case $k = 0$:

$$h \sum_{j\in\mathbb{Z}} u(jh) = \sum_{m\in\mathbb{Z}} \hat{u}(\frac{2\pi}{h}m).$$

Exercise: use what we have already seen concerning translations and Fourier transforms to show that the above equation implies (hence is equivalent to) equation (7.1).

*Proof.* Consider the right-hand side in (7.1), and call it

$$\hat{\phi}(k) = \sum_{m\in\mathbb{Z}} \hat{u}(k + m\frac{2\pi}{h}), \qquad k \in [-\pi/h, \pi/h].$$

It suffices to show that $\hat{\phi}(k) = \hat{v}(k)$, or equivalently in terms of their ISFT, that $\phi_j = v_j$ for $j \in \mathbb{Z}$. The ISFT is written

$$\phi_j = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} \left[ \sum_{m\in\mathbb{Z}} \hat{u}(k + m\frac{2\pi}{h}) \right] e^{ikjh}\, dk.$$

The function $u$ is smooth, hence integrable, and the sum over $m$ converges fast. So we can interchange sum and integral:

$$\phi_j = \frac{1}{2\pi} \sum_{m \in \mathbb{Z}} \int_{-\pi/h}^{\pi/h} \hat{u}(k + m\frac{2\pi}{h}) e^{ikjh}\, dk.$$

Now put $k' = k + m\frac{2\pi}{h}$, and change variable:

$$\phi_j = \frac{1}{2\pi} \sum_{m \in \mathbb{Z}} \int_{-\frac{\pi}{h} - m\frac{2\pi}{h}}^{\frac{\pi}{h} - m\frac{2\pi}{h}} \hat{u}(k') e^{ik'jh} e^{-i\frac{2\pi}{h}jh}\, dk'.$$

The extra exponential factor $e^{-i\frac{2\pi}{h}jh}$ is equal to 1 because $j \in \mathbb{Z}$. We are in presence of an integral over $\mathbb{R}$ chopped up into pieces corresponding to sub-intervals of length $2\pi/h$. Piecing them back together, we get

$$\phi_j = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{u}(k') e^{ik'jh} dk',$$

which is exactly the inverse FT of $\hat{u}$ evaluated at $x_j = jh$, i.e., $\phi_j = u(x_j) = v_j$.

The Poisson summation formula shows that sampling a function at rate $h$ corresponds to periodizing its spectrum (Fourier transform.) with a period $2\pi/h$. So the error made in sampling a function (and subsequently doing bandlimited interpolation) is linked to the possible overlap of the Fourier transform upon periodization.

- **Scenario 1**. Assume $\text{supp}(\hat{u}) \subset [-\pi/h, \pi/h]$. Then no error is made in sampling and interpolating $u$ at rate $h$, because nothing happens upon $2\pi/h$-periodization and windowing into $[-\pi/h, \pi/h]$:

  $$\hat{p}(k) = \hat{u}(k) \qquad \Rightarrow \qquad p(x) = u(x).$$

  (Draw picture)

- **Scenario 2**. Now assume that $\hat{u}(k)$ is not included in $[-\pi/h, \pi/h]$. In general the periodization of $\hat{u}(k)$ will result in some overlap inside $[-\pi/h, \pi/h]$. We call this *aliasing*. In that case, some information is lost and interpolation will not be exact.

Scenario 1 is known as the *Shannon sampling theorem*: a function bandlimited in $[-\pi/h, \pi/h]$ in $k$ space is perfectly interpolated by bandlimited interpolation, on a grid of spacing $h$ or greater. In signal processing $h$ is also called the sampling rate, because $x$ has the interpretation of time. When $h$ is the largest possible rate such that no aliasing occurs, it can be referred to as the Nyquist rate.

More generally, the accuracy of interpolation is linked to the smoothness of $u(x)$. If the tails $\hat{u}(k)$ are small and $h$ is large, we can expect that the error due to periodization and overlap won't be too big. The following result is a consequence of the Poisson summation formula.

**Theorem 15.** *(Error of bandlimited interpolation) Let $u$ have $p \geq 1$ derivatives in $L^1(\mathbb{R})$. Let $v_j = u(x_j)$ at $x_j = jh$, $j \in \mathbb{Z}$. Denote by $p(x)$ the bandlimited interpolant formed form $v_j$. Then, as $h \to 0$,*

$$|\hat{u}(k) - \hat{p}(k)| = O(h^p) \qquad |k| \leq \frac{\pi}{h},$$

*and*

$$\|u - p\|_2 = O(h^{p-1/2}).$$

*Proof.* Denote by $\hat{u}(k)$ the FT of $u(x)$, and by $\hat{v}(k)$ the SFT of $v_j$, so that $\hat{p}(k) = \hat{v}(k)$ on $[-\pi/h, \pi/h]$. By the Poisson summation formula (7.1),

$$\hat{v}(k) - \hat{u}(k) = \sum_{m \neq 0} \hat{u}(k + m\frac{2\pi}{h}), \qquad k \in [-\pi/h, \pi/h].$$

As we saw earlier, the smoothness condition on $u$ imply that

$$|\hat{u}(k)| \leq C\,|k|^{-p}.$$

Since

$$k + m\frac{2\pi}{h} \in [-\frac{\pi}{h} + m\frac{2\pi}{h}, \frac{\pi}{h} + m\frac{2\pi}{h}],$$

we have $|k + m\frac{2\pi}{h}| \geq |m\frac{\pi}{h}|$, hence

$$|\hat{u}(k + m\frac{2\pi}{h})| \leq C'\,|m\frac{\pi}{h}|^{-p},$$

for some different constant $C'$. Summing over $m \neq 0$,

$$|\hat{v}(k) - \hat{u}(k)| \leq C' \sum_{m \neq 0} |m|^{-p} (\frac{\pi}{h})^{-p} \leq C''\,(\frac{\pi}{h})^{-p} \leq C'''\,h^p.$$

One can switch back to the $x$ domain by means of the Plancherel formula

$$\|u - p\|_{L^2}^2 = \frac{1}{2\pi} \|\hat{u}(k) - \hat{v}(k)\|_{L^2(\mathbb{R})}^2.$$

The right-hand side contains the integral of $|\hat{u}(k) - \hat{v}(k)|^2$ over $\mathbb{R}$. Break this integral into two pieces:

- Over $[-\pi/h, \pi/h]$, we have seen that $|\hat{u}(k) - \hat{v}(k)|^2 = O(h^{2p})$. The integral is over an interval of length $O(1/h)$, hence the $L^2$ norm squared is $O(h^{2p-1})$. Taking a square root to get the $L^2$ norm, we get $O(h^{p-1/2})$.
- For $|k| \geq \pi/h$, we have $\hat{p}(k) = 0$, so it suffices to bound $\int_{|k| \geq \pi/h} |\hat{u}(k)|^2 \, dk$. Since $|\hat{u}(k)| \leq C \, |k|^{-p}$, this integral is bounded by $O((\pi/h)^{2p-1})$. Taking a square root, we again obtain a $O(h^{p-1/2})$.

□

We have seen how to interpolate a function defined on $\mathbb{R}$, but as a closing remark let us notice that a similar notion exists for functions defined on intervals, notably $x \in [-\pi, \pi]$ or $[0, 2\pi]$. In that case, wavenumbers are discrete, the FT is replaced by the FS, and the SFT is replaced by the DFT. Evaluating the DFT for $x$ not on the grid would give an interpolant:

$$\frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} e^{ikx} \hat{f}_k.$$

Contrast with the formula (6.8) for the IDFT. This is almost what we want, but not quite, because the highest wavenumber $k = N/2$ is treated asymmetrically. It gives rise to an unnatural complex term, even if $\hat{f}_k$ is real and even. To fix this, it is customary to set $\hat{f}_{-N/2} = \hat{f}_{N/2}$, to extend the sum from $-N/2$ to $N/2$, but to halve the terms corresponding to $k = -N/2$ and $N/2$. We denote this operation of halving the first and last term of a sum by a double prime after the sum symbol:

$$\sum{}''$$

Itis easy to check that this operation does not change the interpolating property. The definition of bandlimited interpolant becomes the following in the case of intervals.

**Definition 22.** *(Spectral interpolation on $[0, 2\pi]$) Let $x_j = jh$, $j = 0, \ldots, N-1$ with $h = 1/N$. Consider $f : [0, 2\pi] \mapsto \mathbb{R}$, its restriction $f_j = f(x_j)$, and the DFT $\hat{f}_k$ of the samples $f_j$. Then the spectral interpolant is*

$$p(x) = \frac{1}{2\pi} {\sum}''^{N/2}_{k=-N/2} e^{ikx} \hat{f}_k.$$

Because $p(x)$ is a superposition of "monomials" of the form $e^{ikx} = (e^{ix})^k$ for $k$ integer, we call it a *trigonometric polynomial.*

The theory for interpolation by trigonometric polynomials (inside $[0, 2\pi]$) is very similar to that for general bandlimited interpolants. The only important modification is that $[0, 2\pi]$ is a periodized interval, so a function qualifies as smooth only if it connects smoothly across $x = 0$ indentified with $x = 2\pi$ by periodicity. The Poisson summation formula is still the central tool, and has a counterpart for Fourier series.

**Theorem 16.** *(Poisson summation formula, FS version) Let $u : [0, 2\pi] \mapsto \mathbb{R}$, sufficiently smooth. Let $v_j = u(\theta_j)$ for $\theta_j = jh$, $j = 1, \ldots, N$, $h = 2\pi/N$, and*

$$\hat{u}_k = \int_0^{2\pi} e^{-ik\theta} u(\theta)\, d\theta, \qquad (FS), \qquad k \in \mathbb{Z},$$

$$\hat{v}_k = h \sum_{j=1}^{N} e^{-ik\theta_j} u(\theta_j). \qquad (DFT), \qquad k = -\frac{N}{2}, \ldots, \frac{N}{2} - 1.$$

*Then*

$$\hat{v}_k = \sum_{m \in \mathbb{Z}} \hat{u}_{k+mN}, \qquad k = -\frac{N}{2}, \ldots, \frac{N}{2} - 1. \tag{7.2}$$

*(Recall that $N = \frac{2\pi}{h}$ so this formula is completely analogous to (7.1).)*

For us, the important consequence is that if $u$ has $p$ derivatives in $L^1$, over the periodized interval $[0, 2\pi]$, then the bandlimited interpolation error is a $O(h^p)$ in the pointwise sense in $k$ space, and $O(h^{p-1/2})$ in the $L^2$ sense.

For this result to hold it is important that $u$ has $p$ derivatives at the origin as well (identified by periodicity with $2\pi$), i.e., the function is equally smooth as it straddles the point where the interval wraps around by periodicity.Otherwise, if $u(\theta)$ has discontinuities such as. $u(2\pi^-) \neq u(0^+)$, interpolation will suffer from the Gibbs effect.

### 7.1.2 Chebyshev interpolation

Consider now smooth functions inside $[-1, 1]$ (for illustration), but not necessarily periodic. So the periodization $\sum_j f(x + 2j)$ may be discontinuous. Polynomial interpolation on equispaced points may fail because of the Runge phenomenon, and bandlimited interpolation will fail due to Gibbs's effect.

A good strategy for interpolation is the same trick as the one we used for truncation in the last chapter: pass to the variable $\theta$ such that

$$x = \cos\theta.$$

Then $x \in [-1, 1]$ corresponds to $\theta \in [0, \pi]$. We define $g(\theta) = f(\cos\theta)$ with $g$ $2\pi$-periodic and even.

We can now consider the bandlimited interpolant of $g(\theta)$ on an equispaced grid covering $[0, 2\pi]$, like for instance

$$\theta_j = \frac{\pi j}{N}, \quad \text{where } j = 1, \ldots, 2N.$$

Using the definition we saw at the end of the last section (with the "double prime"), we get

$$q(\theta) = \frac{1}{2\pi} {\sum}'^{N}_{k=-N} e^{ik\theta} \hat{g}_k, \qquad \hat{g}_k = \frac{\pi}{N} \sum_{j=0}^{2N-1} e^{-ik\theta_j} g(\theta_j).$$

By even symmetry in $\theta$ and $k$ (why?), we can write

$$q(\theta) = \sum_{k=0}^{N} \cos(k\theta) c_k,$$

for some coefficients $c_k$ that are formed from the samples $g(\theta_j)$.

Back to $x$, we get the sample points $x_j = \cos(\theta_j)$. They are called *Chebyshev points*. They are not equispaced anymore, and becauset they are the projection on the $x$-axis of equispaced points on the unit circle, they cluster near the edges of $[-1, 1]$. There are $N+1$ of them, from $j = 0$ to $N$, because of the symmetry in $\theta$. It turns out that the $x_j$ are the *extremal points* of the Chebyshev polynomial $T_N(x)$, i.e., the points in $[-1, 1]$ where $T_N$ takes its maximum and minimum values.

In terms of the variable $x$, the interpolant can be expressed as

$$p(x) = q(\text{acos } x) = \sum_{n=0}^{N} T_n(x) c_n, \qquad T_n(x) = \cos(n \,\text{acos } x),$$

with the same $c_n$ as above. Since $T_n(x)$ are polynomials of degree $0 \le n \le N$, and $p(x)$ interpolates $f(x)$ at the $N+1$ (non-equispaced) points $x_j$, we are in presence of the Lagrange interpolation polynomial for $f$ at $x_j$!

Now, the interesting conclusion is not so much the new formula for the interpolation polynomial in terms of $T_n$, but that although this is a polynomial interpolant, the error analysis is inherited straight from Fourier analysis. If $f$ is smooth, then $g$ is smooth and periodic, and we saw that the bandlimited interpolant converges very fast. The Chebyshev interpolant of $f$ is equal to the bandlimited interplant of $g$ so it converges at the exact same rate (in $L^\infty$ in $k$ or $n$ space) — for instance $O(N^{-p-1})$ when $f$ has $p$ derivatives (in BV).

In particular, we completely bypassed the standard analysis of error of polynomial interpolation, and proved universal convergence for smooth $f$. The factor

$$\pi_{N+1}(x) = \prod_{j=0}^{N} (x - x_j)$$

that was posing problems in the error estimate then does not pose a problem anymore, because of the very special choice of Chebyshev points $\cos(\pi j/N)$ for the interpolation. Intuitively, clustering the grid points near the edges of the interval $[-1, 1]$ helps giving $\pi_{N+1}(x)$ more uniform values throughout $[-1, 1]$, hence reduces the gross errors near the edges.

Let us now explain the differences in the behavior of the monic polynomial $\prod_{j=0}^{N}(x-x_j)$ for equispaced vs. Chebyshev points, and argue that Chebyshev points are near-ideal for interpolation of smooth functions in intervals. The discussion below is mostly taken from Trefethen, p.43. (See also the last problem on homework 2 for an example of different analysis.)

Let $p(z) = \prod_{j=0}^{N}(z - x_j)$, where we have extended the definition of the monic polynomial to $z \in \mathbb{C}$. We compute

$$\log |p(z)| = \sum_{j=0}^{N} \log |z - x_j|,$$

Put

$$\phi_N(z) = (N+1)^{-1} \sum_{j=0}^{N} \log|z - x_j|.$$

The function $\phi_N$ is like an electrostatic potential, due to charges at $z = x_j$, each with potential $(N+1)^{-1}\log|z-x_j|$. Going back to $p(z)$ from $\phi_N$ is easy:

$$p(z) = e^{(N+1)\phi_N(z)}.$$

Already from this formula, we can see that small variations in $\phi_N$ will lead to exponentially larger variations in $p(z)$, particularly for large $N$.

Let us now take a limit $N \to \infty$, and try to understand what happens without being too rigorous. What matters most about the Chebyshev points is their *density*: the Chebyshev points are the projection onto the real-axis of a sequence of equispaced points on a circle. If the density of points on the circle is a constant $1/(2\pi)$, then the density of points on $[-1, 1]$ generated by vertical projection is

$$\rho_{Cheb}(x) = \frac{1}{\pi\sqrt{1-x^2}}. \qquad \text{(normalized to integrate to 1 on } [-1,1])$$

(This is a density in the sense that

$$N \int_a^b \rho_{Cheb}(x)\, dx$$

approximately gives the number of points in $[a, b]$.) Contrast with a uniform distribution of points, with density

$$\rho_{equi}(x) = \frac{1}{2}.$$

Then the potential corresponding to any given $\rho(x)$ is simply

$$\phi(z) = \int_{-1}^{1} \rho(x) \log|z - x|\, dx.$$

The integral can be solved explicitly for both densities introduced above:

- For $\rho_{equi}$, we get

  $$\phi_{equi}(z) = -1 + \frac{1}{2} Re((z+1)\log(z+1) - (z-1)\log(z-1)).$$

  It obeys $\phi_{equi}(0) = -1$, $\phi_{equi}(\pm 1) = -1 + \log 2$.

- For $\rho_{Cheb}$, we get

$$\phi_{Cheb}(z) = \log \frac{|z - \sqrt{z^2-1}|}{2}.$$

  This function obeys (interesting exercise) $\phi_{Cheb}(x) = -\log 2$ for all $x \in [-1,1]$ on the real axis.

The level curves of both $\phi_{equiv}$ and $\phi_{Cheb}$ in the complex plane are shown on page 47 of Trefethen.

Overlooking the fact that we have passed to a continuum limit for the potentials, we can give a precise estimate on the monic polynomial:

$$|p_{equi}(z)| \simeq e^{(N+1)\phi_{equi}(z)} = \begin{cases} (2/e)^N & \text{near } x = \pm 1; \\ (1/e)^N & \text{near } x = 0. \end{cases}$$

whereas

$$|p_{Cheb}(z)| \simeq e^{(N+1)\phi_{equi}(z)} = 2^{-N}, \qquad z \in [-1,1].$$

We see that $p_{equi}$ can take on very different values well inside the interval vs. near the edges. On the other hand the values of $p_{Cheb}$ are near-constant in $[-1,1]$. The density $\rho_{Cheb}(x)$ is the only one that will give rise to this behavior, so there is something special about it. It is the difference in asymptotic behavior of $(2/e)^{-N}$ vs. $2^{-N}$ that makes the whole difference for interpolation, as $N \to \infty$.

One may argue that neither $p_{equi}$ nor $p_{Cheb}$ blow up as $N \to \infty$, but it is an interesting exercise to show that if we were interpolating in an interval $[-a,a]$ instead of $[-1,1]$, then the bounds would be multiplied by $a^N$, by homogeneity.

The Chebyshev points are not the only one that correspond to the density $\rho_{Cheb}(x)$ as $N \to \infty$. For instance, there is also the Chebyshev roots

$$\theta'_j = \frac{\pi}{2N} + \frac{\pi j}{N}, \qquad j = 0, \ldots, 2N-1,$$

which are the *roots* of $T_N(x)$, instead of being the extremal points. They give rise to very good interpolation properties as well.

Finally, let us mention that the theory can be pushed further, and that the exponential rate of convergence of Chebyshev interpolation for analytic functions can be linked to the maximum value of $\phi(z)$ on the strip in which the extension $f(z)$ of $f(x)$ is analytic. We will not pursue this further.

## 7.2 Differentiation

### 7.2.1 Bandlimited differentiation

The idea that a numerical approximation of a derivative can be obtained from differentiating an interpolant can be pushed further. In this section we return to bandlimited interpolants. We've seen that they are extremely accurate when the function is smooth and periodic; so is the resulting differentiation scheme. It is called bandlimited differentiation, or spectral differentiation.

First consider the case of $x \in \mathbb{R}$ and $x_j = jh$, $j \in \mathbb{Z}$. As we've seen, the bandlimited/spectral interpolant of $u(x_j)$ is

$$p(x) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{ikx} \hat{u}(k)\, dk,$$

where $\hat{v}(k)$ is the SFT of $v_j = u(x_j)$. Differentiating $p(x)$ reduces to a multiplication by $ik$ in the Fourier domain. Evaluating $p'(x_j)$ is then just a matter of letting $x = x_j$ in the resulting formula. The sequence of steps for bandlimited differentiation ($x \in \mathbb{R}$) is the following:

- Obtain the SFT $\hat{v}(k)$ of $v_j = u(x_j)$;
- Multiply $\hat{v}(k)$ by $ik$;
- Obtain the ISFT of $\hat{w}(k) = ik\hat{v}(k)$, call it $w_j$.

The numbers $w_j$ obtained above are an approximation of $u'(x_j)$. The following result makes this precise.

**Theorem 17.** *(Accuracy of bandlimited differentiation, see also Theorem 4 in Trefethen's book) Let $u$ have $p$ derivatives in $L^1(\mathbb{R})$. Let $v_j = u(x_j)$, and $w_j = p'(x_j)$ be the result of bandlimited differentiation. Then*

$$\sup_j |w_j - u'(x_j)| = O(h^{p-2}).$$

*and*

$$\|u' - p'\|_2 = O(h^{p-3/2}).$$

*Proof.* The proof hinges on the fact that

$$|\hat{v}(k) - \hat{u}(k)| = O(h^p).$$

One power of $h$ is lost when differentiating $u$ (because $ik$ is on the order of $1/h$ over the fundamental cell $[-\pi/h, \pi/h]$). Half a power of $h$ is lost in going back to the physical domain ($j$ instead of $k$) via the $L^2$ norm (why?), and a full power of $h$ is lost when going back to $j$ in the uniform sense (why?). □

The point of the above theorem is that the order of bandlimited differentiation is directly linked to the smoothness of the function, and can be arbitrarily large. This is called spectral accuracy. One can even push the analysis further and show that, when $f$ is real-analytic, then the rate of convergence of $w_j$ towards $u'(x_j)$ is in fact exponential/geometric.

Of course in practice we never deal with a function $u(x)$ defined on the real line. In order to formulate an algorithm, and not simply a sequence of abstract steps, we need to limit the interval over which $u$ is considered. Spectral differentiation in the periodic interval $[0, 2\pi]$ works like before, except DFT are substituted for SFT. For $\theta \in [0, 2\pi]$, we've seen that the spectral interpolant is defined as

$$p(\theta) = \frac{1}{2\pi} {\sum}''^{N/2}_{k=-N/2} e^{ik\theta} \hat{f}_k.$$

(The double prime is important here.) Again, a derivative can be implemented by multiplying by $ik$ in the Fourier domain. The sequence of steps is very similar to what it was before, except that we can now label them as "compute", and not just "obtain":

- Compute the DFT $\hat{v}_k$ of $v_j = u(x_j)$;
- Multiply $\hat{v}_k$ by $ik$;
- Compute the IDFT of $\hat{w}_k = ik\hat{v}_k$, call it $w_j$.

The result of accuracy are the same as before, with the provision that $u$ needs to be not only smooth, but also smooth when extended by periodicity.

The FFT can be used to yield a fast $O(N \log N)$ algorithm for spectral differentiation.

Note that higher derivatives are obtained in the obvious manner, by multiplying in Fourier by the adequate power of $ik$.

### 7.2.2 Chebyshev differentiation

In view of what has been covered so far, the idea of Chebyshev differentiation is natural: it is simply differentiation of the Chebyshev interpolant at the Chebyshev nodes. It proves very useful for those smooth functions on an interval, which do not necessarily extend smoothly by periodicity.

Let us recall that the Chebyshev interpolant is $q(x) = p(\arccos x)$, where $p(\theta)$ is the bandlimited interpolant of $u(\cos \theta_j)$ at the Chebyshev points $x_j = \cos \theta_j$. As such, a differentiation on $q(x)$ is not the same thing as a differentiation on $p(\theta)$. Instead, by the chain rule,

$$q'(x) = \frac{-1}{\sqrt{1-x^2}} p'(\arccos x).$$

The algorithm is as follows. Start from the knowledge of $u(x_j)$ at $x_j = \cos \theta_j$, $\theta_j = jh$, $h = \pi/N$, and $j = 1, \ldots, N$.

- Perform an even extension of $u(x_j)$ to obtain $u(\cos \theta_j)$ for $\theta_j = jh$, $h = \pi/N$, and $j = -N+1, \ldots, N$. Now we have all the equispaced sample of the periodic function $u(\cos \theta)$ for $\theta_j$ covering $[0, 2\pi]$, not just $[0, \pi]$.

- Take the DFT of those samples, call it $\hat{v}_k$,

- Multiply by $ik$,

- Take the IDFT of the result $ik\hat{v}_k$,

- Multiply by $-1/\sqrt{1-x_j^2}$ to honor the chain rule. At the endpoints $x_j = -1$ or $1$, take a special limit to obtain the proper values of $p'(-1)$ and $p(1)$. See Trefethen's book for the correct values.

This is a fast algorithm since we can use the FFT for the DFT and IDFT.

Since we are only a change of variables away from Fourier analysis in a periodic domain, the accuracy of Chebyshev differentiation is directly inherited from that of bandlimited differentiation. We also have spectral accuracy.

Note that higher derivatives can be treated similarly, by applying the chain rule repeatedly.

In practice, Chebyshev methods are particularly useful for boundary-value problems (we'll come back to this), when all samples of a function are to be determined at once, and when we have the freedom of choosing the sample points.

# 7.3 Integration

## 7.3.1 Spectral integration

To go beyond methods of finite order, the idea of spectral integration is to integrate a bandlimited interpolant. This strategy yields very high accuracy when the function is smooth and periodic.

Consider a function $u(\theta)$, $\theta \in [0, 2\pi]$. Its samples are $v_j = u(\theta_j)$ with $\theta_j = jh$, $h = 2\pi/N$, and $j = 1, \ldots, N$. Form the DFT:

$$\hat{v}_k = h \sum_{j=1}^{N} e^{-ik\theta_j} v_j,$$

and the bandlimited interpolant,

$$p(\theta) = \frac{1}{2\pi} \sum\nolimits''^{N/2}_{k=-N/2} e^{ik\theta} \hat{v}_k.$$

Integrating $p(\theta)$ gives the remarkably simple following result.

$$\int_0^{2\pi} p(\theta)\, d\theta = \hat{v}_0 = h \sum_{j=1}^{N} u(\theta_j).$$

We are back to the trapezoidal rule! (The endpoints are identified, $\theta_0 = \theta_N$.) While we have already encountered this quadrature rule earlier, it is now derived from Fourier analysis. So the plot thickens concerning its accuracy properties.

Specifically, we have to compare $\hat{v}_0$ to $\hat{u}_0 = \int_0^{2\pi} u(\theta)\, d\theta$, where $\hat{u}_k$ are the Fourier series coefficients of $u(\theta)$. The relationship between $\hat{v}_0$ and $\hat{u}_0$ is the Poisson summation formula (7.2):

$$\hat{v}_0 = \sum_{m \in \mathbb{Z}} \hat{u}_{mN}, \qquad N = \frac{2\pi}{h}.$$

The most important term in this sum is $\hat{u}_0$ for $m = 0$, and our task is again to control the other ones, for $m \neq 0$. The resulting accuracy estimate is the following.

**Theorem 18.** *Assume $u$ has $p$ derivatives in $L^1[0,2\pi]$, where $[0,2\pi]$ is considered a periodic interval. (So it matters that the function connects smoothly by periodicity.) Then*

$$\int_0^{2\pi} u(\theta)\, d\theta - h\sum_{j=1}^{N} u(\theta_j) = O(h^p).$$

*Proof.* By the Poisson summation formula, in the notations of the preceding few paragraphs,

$$\hat{u}_0 - \hat{v}_0 = \sum_{m\neq 0} \hat{u}_{mN}.$$

We have already seen that the smoothness properties of $u$ are such that

$$|\hat{u}_k| \leq C|k|^{-p}.$$

So we have

$$|\hat{u}_0 - \hat{v}_0| \leq C \sum_{m\neq 0} (mN)^{-p} \leq C'\, N^{-p},$$

which is a $O(h^p)$. □

As a conclusion, the trapezoidal rule is spectrally accurate (error $O(h^{p+1})$ for all $p \geq 0$ when $u \in C^\infty$), *provided* the function to be integrated in smooth *and* periodic. If the function is $C^\infty$ in an interval but is for instance discontinuous upon periodization, then we revert to the usual $O(h^2)$ rate. So the true reason for the trapezoidal rule generally being $O(h^2)$ and not $O(h^\infty)$ is only the presence of the boundaries!

An important example of such periodic smooth function, is a regular $C^\infty$function multiplied by a $C^\infty$ window that goes smoothly to zero at the endpoints of $[a,b]$, like for instance a member of a partition of unity. (This plays an important role in some electromagnetism solvers, for computing the radar cross-section of scatterers.)

### 7.3.2 Chebyshev integration

Like for Chebyshev differentiation, we can warp $\theta$ into $x$ by the formula $\theta = \arccos x$, and treat smooth functions that are not necessarily periodic. Integrating a Chebyshev interpolant gives rise to Chebyshev integration, also called Clenshaw-Curtis quadrature.

Assume that $f(x)$ is given for $x \in [-1,1]$, otherwise rescale the $x$ variable. The Chebyshev interpolant is built from the knowledge of $f$ at the Chebyshev nodes $x_j = \cos\theta_j$, and takes the form

$$p(x) = \sum_{n \geq 0} a_n T_n(x).$$

We have seen that $a_n$ are obtained by even extension of $f(x_j)$, followed by an FFT where the sine terms are dropped. As a result,

$$\int_{-1}^{1} p(x)\,dx = \sum_{n\geq 0} a_n \int_{-1}^{1} T_n(x)\,dx.$$

We compute

$$\int_{-1}^{1} T_n(x)\,dx = \int_{0}^{\pi} \cos(n\theta)\sin\theta d\theta.$$

This integral can be evaluated easily by relating cos and sin to complex exponentials (or see Trefethen's book for an elegant shortcut via complex functions), and the result is

$$\int_{-1}^{1} T_n(x)\,dx = \begin{cases} 0 & \text{if } n \text{ is odd;} \\ \frac{2}{1-n^2} & \text{if } n \text{ is even.} \end{cases}$$

The algorithm for Chebyshev differentiation is simply: (1) find the coefficients $a_n$ for $0 \leq n \leq N$, and (2) form the weighted sum

$$\sum_{n \text{ even}, n\leq N} a_n \frac{2}{1-n^2}.$$

The accuracy estimate of Chebyshev integration is the same as that of bandlimited integration, except we do not need periodicity. So the method is spectrally accurate.

An important method related to Chebyshev quadrature is Gaussian quadrature, which is similar but somewhat different. It is also spectrally accurate for smooth functions. Instead of using extrema or zeros of Chebyshev polynomials, it uses zeros of Legendre polynomials. It is usually derived directly from properties of orthogonal polynomials and their zeros, rather than Fourier analysis. This topic is fascinating but would take us a little too far.

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