Quick introduction to PDE

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1 Intro

These are notes for three workshop meetings that cover background material for the class Numerical Methods II. I assume a good undergraduate level background in mathematics, including linear algebra, an idea of an abstract vector space, complex numbers and exponentials, and multi-variate calculus.

2 Fourier series

Suppose $u(x)$ is a periodic function of x with period L. This means that $u(x+L) = u(x)$ for all x. Examples of periodic functions are: constants, $\sin(2\pi x/L)$, $\cos(2\pi x/L)$, $\sin(4\pi x/L)$, etc. A *Fourier series* representation of a periodic function is a formula that expresses the function as a sum of these basic periodic functions:

$$
\begin{aligned}
u(x) &= \alpha_0 + \alpha_1 \cos(2\pi x/L) + \beta_1 \sin(2\pi x/L) + \alpha_2 \cos(4\pi x/L) + \cdots \\
u(x) &= \sum_{k=0}^{\infty} \alpha_k \cos(2\pi k x/L) + \sum_{k=1}^{\infty} \beta_k \sin(2\pi k x/L) \; . \qquad (1)
\end{aligned}
$$

This expresses $u(x)$ in terms of sines and cosines of higher and higher frequency as $k \to \infty$. Naturally, you should ask:

1. Is this possible?
2. If it is possible, how do you do it?
3. Why do it?
   - What do we learn about u from its *Fourier coefficients* α_k and β_k?
   - What can you learn about differential equations using Fourier series?
   - What numerical algorithms rely on Fourier series?

These notes focus on the "how" with only a little on the "why".

The algebra is simpler using complex exponentials instead of line and cosine. This is possible because of the Euler formula

$$
e^{i\theta} = \cos(\theta) + i \sin(\theta) \; . \qquad (2)
$$

With some algebra, this leads to

$$
\cos(\theta) = \frac{e^{i\theta} + e^{-i\theta}}{2} \qquad (3)
$$

$$
\sin(\theta) = \frac{e^{i\theta} - e^{-i\theta}}{2i} \qquad (4)
$$

Now, write $\theta = 2\pi kx/L$ and substitute into the series (1) and you get an equivalent representation using possibly complex Fourier coefficients

$$u(x) = \sum_{k=-\infty}^{\infty} a_k e_k(x) \; , \tag{5}$$

with

$$e_k(x) = e^{2\pi ix/L} \tag{6}$$

The real Fourier sine and cosine series has mode number k running from 0 or 1 to infinity without using negative k. The complex exponential Fourier series (5) (6) requires positive and negative k. This is because the representation formulas (3) and (4) require $e^{2\pi 2kx/L}$ and $e^{-2\pi ikx/l}$ to represent $\cos(2\pi kx/L)$.

You can think of Fourier series as representing a periodic function as a linear combination of *basis functions* that are *Fourier modes*. The periodic function u is an element of some vector space and the Fourier modes e_k are a basis for that space. The Fourier sum (5) represents u as a linear combination of basis vectors. The vector space in "infinite dimensional" because there are infinitely many linearly independent basis vectors.

The Fourier coefficients a_k may not be real even when the target function u is real. Fourier analysis is often done with complex arithmetic. This is true even in the computer, where u is replaced by a vector with finitely many components and the sum is the *DFT* (for Discrete Fourier Transform). In that case, the algorithm that computes the discrete Fourier coefficients is the *Fast Fourier Transform* or *FFT*. The FFT packages in Matlab or Python produce complex numbers a_k when presented with real numbers u_j. For that reason, we work with complex vector spaces.

Most readers will have seen some of this material before, but the notation and precise terminology may have been different. There are many different but equivalent ways to describe Fourier series and integrals. Whenever someone uses Fourier analysis, you may have to force them to give the precise definitions they're using.

Abstract real and complex vector space

A *vector space* is a collection of "objects" that can be added and multiplied by "scalars" (numbers). Specifically, suppose a and b are numbers and u and v are vectors, then $u + v$ (vector addition) and au (scalar multiplication) are defined and satisfy the usual laws for these operations, being commutative (i.e., $u + v = v + u$), associative (i.e., $u + (v + w) = (u + v) + w$, and $(ab)u = a(bu)$), distributive (i.e., $a(u + v) = au + av$, and $(a + b)u = au + bu$), etc. A vector space is *real* or *complex* depending on whether the scalars are real or complex numbers.

An *inner product* on a complex vector space is an operation that produces a complex number from two vectors. The operation should be *bilinear*. For complex vector spaces, this means additive in the vectors, linear or *anti-linear* in the scalars, "conjugate symmetric" (dunno the official term) under vector exchange, and positive definite. If $z = x + iy$ is a complex number, the complex conjugate is $\overline{z} = x - iy$, the square norm is $|z|^2 = \overline{z}z = x^2 + y^2$, and the real part is $2x = 2\mathrm{Re}(z) = \overline{z} + z$.

$$
\begin{array}{rll}
\langle u, v\rangle = & \text{a complex number, the } \textit{scalar product} \text{ of } u \text{ and } v & \\
\langle u + w, v\rangle = \langle u, v\rangle + \langle w, v\rangle & \text{(additive in the first argument – also the second)} \\
\langle u, v\rangle = \overline{\langle v, u\rangle} & \text{(conjugate symmetric)} \\
\langle au, v\rangle = \overline{a}\,\langle u, v\rangle & \text{(anti-linear in the first argument)} \\
\langle u, av\rangle = a\,\langle u, v\rangle & \text{(linear in the second argument)} \\
\langle u, u\rangle > 0 \quad \text{if } u \neq 0 & \text{(positive definite)}
\end{array}
$$

The *norm* of a vector is defined using the inner product as $\|u\| = \langle u, u\rangle^{\frac{1}{2}}$. For practice with these notations, here is a proof of the *Cauchy Schwarz inequality*

$$
|\langle u, v\rangle| \leq \|u\|\,\|v\| \ . \tag{7}
$$

This depends on the inner product being positive definite, which implies that for any complex number a,

$$
\langle u + av, u + av\rangle \geq 0 \ .
$$

The proof chooses a to make the left side small, but it cannot be smaller than zero. Expanding out using additivity, etc:

$$
\begin{aligned}
\langle u + av, u + av\rangle &= \langle u, u\rangle + \langle av, u\rangle + \langle u, av\rangle + \langle av, av\rangle \\
&= \|u\|^2 + \overline{\langle u, av\rangle} + \langle u, av\rangle + \overline{a}a\langle v, v\rangle \\
&= \|u\|^2 + 2\,\mathrm{Re}(\,a\,\langle u, v\rangle) + |a|^2\,\langle v, v\rangle \quad \geq 0 \ .
\end{aligned}
$$

A trick that makes this expression "more real" is to take the complex number a to be $a = t\overline{\langle u, v\rangle}$, with a real number t. This leads to $2\,\mathrm{Re}(\,a\,\langle u, v\rangle) = 2t\,|\langle u, v\rangle|^2$, because t and $\overline{\langle u, v\rangle}\langle u, v\rangle = |\langle u, v\rangle|^2$ are real, and $|a|^2 = t^2\,|\langle u, v\rangle|^2$. Thus,

$$
0 \leq \langle u + av, u + av\rangle = \|u\|^2 + 2t\,|\langle u, v\rangle|^2 + t^2\,|\langle u, v\rangle|^2\,\|v\|^2 \ .
$$

You minimize over t by differentiating with respect to t, setting the derivative to zero, and solving for t. The result is

$$
t_* = -\frac{1}{\|v\|^2} \ .
$$

Substitute this in, simplify, and you get

$$
0 \leq \|u\|^2\,\|v\|^2 - |\langle u, v\rangle|^2 \ .
$$

This is the Cauchy Schwarz inequality (7).

Spaces of sequences are natural examples of real or complex inner product spaces. The space $\mathbb{C}^n$ is the space of sequences of n complex numbers

$$u = (u_1, \cdots, u_n) \in \mathbb{C}^n \ , \quad u_k \in \mathbb{C} \ .$$

You vector addition and scalar multiplication is “componentwise”. The inner product is

$$\langle u, v\rangle = \sum_{k=1}^{n} \overline{u}_k v_k \ .$$

You can check that this has all the properties of an inner product. [*Warning*, some people prefer to take $u_k\overline{v}_k$ in the inner product. This would make it anti-linear in the second vector, not the first.] Vectors as sequences may be re-interpreted as column vectors

$$u = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} \ .$$

In that case, the conjugate transpose is the row vector

$$u^* = (\overline{u}_1, \cdots, \overline{u}_n) \ .$$

In vector notation, the inner product is

$$\langle u, v\rangle = u^* v \ .$$

You have to decide whether $(u_1, \cdots, u_n)$, is a sequence vector or a row vector, as the notation is the same.

Any linear subspace of an inner product space is an inner product space. For example, you could consider the space of sequences whose members add up to zero.

You could also take spaces of infinite sequences that are *square summable.* These are denoted $l^2(I)$, where I represents the indexing used for the sequences. For example, $\mathbb{N} = \{1, 2, \cdots\}$ is the set of natural numbers, so think of *singly infinite* sequences of the form $(u_1, u_2, \cdots)$. Such a sequence is in $l^2(\mathbb{N})$ if

$$\|u\|^2 = \sum_{k=1}^{\infty} |u_k|^2 < \infty \ . \tag{8}$$

The inner product is

$$\langle u, v\rangle = \sum_{k=1}^{\infty} \overline{u}_k v_k \ . \tag{9}$$

The set of all integers is $\mathbb{Z} = \{\cdots, -1, 0, 1, 2, \cdots\}$, and a *doubly infinite sequence* has the form *doubly infinite* sequences of the form $u = (\cdots, u_{-1}, u_0, u_1, u_2, \cdots)$. Such a sequence is in $l^2(\mathbb{Z})$ if

$$\|u\|^2 = \sum_{k=-\infty}^{\infty} |u_k|^2 < \infty \ .$$

The inner product is similar. You might worry that the inner product is an infinite sum that does not converge. Don't worry. The Cauchy Schwarz inequality implies that the inner product sum (9) converges if the norm sums (8) converge for u and v.

The inner product spaces $L^2(\mathcal{S})$ are functions of a continuous variable $x \in \mathcal{S}$. You can think of a sequence as a function of the index, k, so this is similar. The *domain*, $\mathcal{S}$, may be an interval on the real line, or the whole line, or a region of n dimensional space. The space $L^2(\mathcal{S})$, is[1] the set of functions defined for $x \in \mathcal{S}$ with

$$\|u\|^2 = \int_{x\in\mathcal{S}} |u(x)|^2 \, dx < \infty \ .$$

The inner product is

$$\langle u, v\rangle = \int_{x\in\mathcal{S}} \overline{u(x)}\, v(x)\, dx \ .$$

For example, $u \in L^2(\mathbb{R})$ if $u(x)$ is defined for all real numbers x and if

$$\|u\|^2 \ \int_{\infty}^{\infty} |u(x)|^2 \, dx < \infty \ .$$

Again, the Cauchy Schwarz inequality implies that the inner product integral converges if u and v are square integrable.

A function of $x \in \mathbb{R}$ is *periodic* with period L if $u(x + L) = u(x)$ for all x. The corresponding space of square integrable periodic functions is $L^2(\text{per})$. The inner product is

$$\langle u, v\rangle_{\text{per}} = \int_0^L \overline{u}(x) v(x)\, dx \ . \tag{10}$$

The integral is the same if the integration region $[0, L]$ is replaced by any set that covers the same points. For example, you get the same answers using a symmetric interval

$$\langle u, v\rangle_{\text{per}} = \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \overline{u}(x) v(x)\, dx \ .$$

The space $L^2(\text{per})$ is the one that is relevant for Fourier series.

Orthonormal basis

An orthonormal basis for an $n-$dimensional inner product space, V, is a family $e_1, \cdots, e_n$ with the property

$$\langle e_j, e_k\rangle = \delta_{jk} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases} \tag{11}$$

[1]This not strictly true. A class on "real variables" would explain the completely correct version of these definitions using concepts of measurability and almost everywhere.

This δ_{jk} is the *Kronecker symbol*. The numbers δ_{jk} are the entries of the identity matrix. If $u \in V$, it can be represented in terms of the basis. Here are the relevant formulas, which are derived in any (good) linear algebra book

$$
\begin{aligned}
u &= \sum_{k=1}^{n} a_k e_k && (12)\\
a_k &= \langle e_k, u \rangle && (13)\\
\|u\|^2 &= \sum_{k=1}^{n} |a_k|^2 && (14)\\
\langle u, v \rangle &= \sum_{k=1}^{n} \overline{a}_k b_k \ , \quad \text{if } v = \sum_{k=1}^{n} b_k e_k \ . && (15)
\end{aligned}
$$

If V is $n-$dimensional, any basis has n elements. If $e_1, \cdots, e_n$ is an orthonormal family, then they form a basis.

An *infinite dimensional* inner product space is one that does not have a finite basis. The spaces l^2 and L^2 are infinite dimensional in this sense. For finite dimensional spaces, you know the vectors e_k are a basis if they are orthonormal and there are enough of them (n of them). In infinite dimensions it is possible to have infinitely many orthonormal vectors e_k that do not form a basis. For example, if the vectors $e_1, e_2, \cdots$ form a basis, then the set set $e_2, e_3, \cdots$ that leaves out e_1 is not a basis, but it still is an infinite family of orthonormal vectors. A set of orthonormal vectors is *complete* if it forms a basis. A complete family e_k satisfies the formulas (12), (13), (14) and (15), provided you sum over all the k that are the index set for the basis.

Fourier modes

The basic Fourier modes for period $L = 1$ are the functions

$$
e_k(x) = e^{2\pi i x} \ . \qquad (16)
$$

The mode number k can be any integer, positive or negative. These are elements of the inner product space $L^2(\text{per})$ with period $L = 1$, and you can check that $e_k(x+1) = e_k(x)$. Some integration verifies the normalization and orthogonality relations (11). Keep in mind the basic properties of the complex exponential:

$$
\begin{aligned}
e^{i\theta} &= \cos(\theta) + i\sin(\theta)\\
\left|e^{i\theta}\right|^2 &= \cos^2(\theta) + \sin^2(\theta) = 1\\
e^{-i\theta} &= \overline{e^{i\theta}}\\
&\quad (\text{because } e^{-i\theta} = \cos(-\theta) + i\sin(-\theta) = \cos(\theta) - i\sin(\theta) = \overline{\cos(-\theta) + i\sin(-\theta)})\\
\overline{e^{i\theta}}\, e^{i\phi} &= e^{i(\phi-\theta)}\\
e^{2\pi i m} &= 1 \ , \quad \text{if } m \text{ is an integer} \ .
\end{aligned}
$$

For $j = k$ we have

$$\begin{aligned}
\langle e_k, e_k \rangle &= \|e_k\|^2 \\
&= \int_0^1 |e_k(x)|^2 \, dx \\
&= \int_0^1 \left| e^{2\pi i x} \right|^2 \, dx \\
&= \int_0^1 1 \, dx \\
&= 1 \, .
\end{aligned}$$

For $j \neq k$, we use a derivative identity (two forms of it) that applies for any $p \neq 0$:

$$\frac{d}{dx} e^{ipx} = ipe^{ipx} \; , \qquad \frac{1}{ip} \frac{d}{dx} e^{ipx} = e^{ipx} \; . \tag{17}$$

We write $m = k - j$ and note that m is an integer, with $m \neq 0$ when $k \neq j$.

$$\begin{aligned}
\langle e_j, e_k \rangle &= \int_0^1 \overline{e_j(x)} \, e_k(x) \, dx \\
&= \int_0^1 \overline{e^{2\pi i j x}} \, e^{2\pi i k x} \, dx \\
&= \int_0^1 e^{-2\pi i j x} \, e^{2\pi i k x} \, dx \\
&= \int_0^1 e^{2\pi i (k-j) x} \, dx \\
&= \frac{1}{2\pi i m} \int_0^1 \frac{d}{dx} e^{2\pi i m x} \, dx \\
&= \frac{1}{2\pi i m} \left[e^{2\pi i m} - 1 \right] = 0
\end{aligned}$$

This verifies the fact that the Fourier modes satisfy the orthonormality relations (11).

Although these simple calculations verify that the Fourier modes are orthonormal, there is no equally simple way to verify that they are complete. Here are some ways to show that Fourier modes are complete. I may write up the DFT approach later.

- A traditional Fourier series class might use properties of the Fejer kernel.
- Fourier series formulas may be derived from Fourier transform formulas that are verified by may be proven by integral calculations.
- The discrete Fourier modes are complete because there are n of them in an $n-$dimensional space. Fourier series formulas may be proven as $n \to \infty$ limits of DFT (discrete Fourier transform) formulas.

For now, please just accept the fact that Fourier modes are complete.

Now we can rewrite the orthonormal family formulas as formulas involving Fourier modes. The expansion formula (12) is

$$u(x) = \sum_{k=-\infty}^{\infty} a_k e^{2\pi i k x} \; . \tag{18}$$

The sum on the right is the *Fourier series* (an infinite sum may be called a *series*). The formula is the Fourier series representation of the periodic function u. Every term on the right is periodic with period $L = 1$, because k is an integer. Therefore the sum $u(x)$ also has period 1. It is a less obvious theorem that "any" periodic function has a Fourier series representation of this form. That is the completeness theorem for Fourier series.

The numbers a_k are the *Fourier coefficients*. The abstract formula (13) can be written out concretely for Fourier series as

$$a_k = \int_0^1 e^{-2\pi i k x} u(x)\, dx \; . \tag{19}$$

The abstract formula (15) may be written explicitly as

$$\int_0^1 \overline{u}(x) v(x)\, dx = \sum_{k=-\infty}^{\infty} \overline{a}_k b_k \; . \tag{20}$$

In Fourier analysis, this is called the *Parseval* relation.

There are few periodic functions whose Fourier coefficients can be calculated directly. Most of them are variations on the step function defined using a step length r between 0 and 1:

$$u(x) = \begin{cases} 1 & \text{if } 0 \le x \le r \\ 0 & \text{if } r < x < 1 \end{cases}$$

The function u itself is periodic, so, for example, $u(2+\frac{r}{2}) = 1$ and $u(\frac{r}{2} - \frac{1}{2}) = 0$. The Fourier coefficients are

$$\begin{aligned} a_k &= \int_0^r e^{-2\pi i k x}\, dx \\ &= \frac{1}{-2\pi i k} e^{-2\pi i k x} \Big|_0^r \\ &= \frac{1}{2\pi i k} \left[1 - e^{-2\pi i k r} \right] \; . \end{aligned}$$

A particularly simple case is $r = \frac{1}{2}$. Recall the "Euler formula"

$$e^{i\pi(\text{odd integer})} = -1 \; .$$

This gives $a_k = 0$ if k is even and $a_k = \frac{1}{\pi i k}$ if k is odd. These calculations don't apply when $k = 0$, but the $k = 0$ Fourier coefficient is

$$a_0 = \langle e_0, u \rangle = \int_0^1 u(x)\, dx = r \; .$$

It is traditional to use Parseval's formula (20) with this example to derive interesting sum formula. We take $r = \frac{1}{2}$ and $u = v$. The integral on the left is

$$\int_0^1 \left| u(x) \right|^2 \, dx = \frac{1}{2} \; .$$

The sum on the right has only odd k terms, except for $k = 0$, so we write $k = 2j + 1$ The term with k and $-k$ are the same, so we just double the positive k terms. The resulting sum is

$$\left| a_0 \right|^2 + 2 \sum_{j=1}^{\infty} \left| a_{2j+1} \right|^2 = \frac{1}{4} + 2 \sum_{j=1}^{\infty} \frac{1}{\pi^2 (2j+1)^2}$$

Putting these together, with some algebra, leads to

$$\sum_{j=1}^{\infty} \frac{1}{(2j+1)^2} = \frac{\pi^2}{8} \; .$$

This is a famous formula first derived by Euler a different way.

The sine and cosine basis is a possibly more intuitive alternative to the complex exponential basis. The sine and cosine basis functions are

$$\begin{aligned} s_k(x) &= \sin(2\pi k x) \; , \quad k = 1, 2, \cdots \\ c_k(x) &= \cos(2\pi k x) \; , \quad k = 0, 1, 2, \cdots \; . \end{aligned}$$

For each $k > 0$, c_k and s_k span the same two dimensional subspace as e_k and e_{-k}. More plainly, the Euler relation (2) gives

$$\begin{aligned} e_k(x) = e^{2\pi i k x} &= \cos(2\pi k x) + i \sin(2\pi k x) = c_k(x) + i s_k(x) \\ e_{-k}(x) = e^{2\pi i k x} &= \cos(2\pi k x) - i \sin(2\pi k x) = c_k(x) - i s_k(x) \end{aligned}$$

The equivalent formulas (3) and (4) give the reverse relations

$$\begin{aligned} c_k &= \frac{1}{2} e_k + \frac{1}{2} e_{-k} \\ s_k &= \frac{1}{2i} e_k - \frac{1}{2i} e_{-k} \end{aligned}$$

For $k = 0$, the formula is just $c_0 = e_0 = 1$. Therefore, if u has a complex exponential Fourier series representation (18), then it has a sine and cosine representation of the form (1) You can find the coefficients α_k and β_k from the a_k in the complex Fourier series representation. You also can find them from orthogonality relations:

$$\begin{aligned}
\langle c_j, s_k \rangle &= 0 \quad \text{for all } j \text{ and } k \\
\langle s_j, s_k \rangle &= 0 \quad \text{if } j \neq k \\
\langle c_j, c_k \rangle &= 0 \quad \text{if } j \neq k \\
\langle s_j, s_j \rangle &= \frac{1}{2} \quad \text{if } j > 0 \\
\langle c_j, c_j \rangle &= \frac{1}{2} \quad \text{if } j > 0 \\
\langle c_0, c_0 \rangle &= 1 \; .
\end{aligned}$$

If you take the inner product $\langle c_0, u \rangle$ in the sum (1) using these orthogonality relations, you find

$$\alpha_0 = \langle c_0, u \rangle = \int_0^1 u(x)\, dx \; .$$

If you take the inner product $\langle c_j, u \rangle$ or $\langle s_j, u \rangle$ with $j > 0$ in the sum, you find

$$\begin{aligned}
\alpha_j = \langle c_j, u \rangle &= 2 \int_0^1 \cos(2\pi j x)\, u(x)\, dx \\
\beta_j = \langle c_j, u \rangle &= 2 \int_0^1 \sin(2\pi j x)\, u(x)\, dx \; .
\end{aligned}$$

These formulas show that the sine and cosine representation of a real periodic function u involves all real coefficients. You don't need complex vector spaces or even complex numbers to do Fourier sine and cosine series of real periodic functions. The complex version makes the formulas a little simpler (paradox?).

Look at the sine and cosine representation of the step function with $r = \frac{1}{2}$. If k is positive and odd, then the e_k and e_{-k} terms in the complex Fourier expansion are, with $a_k = \frac{1}{2ik}$,

$$\begin{aligned}
a_k e_k(x) + a_{-k} e_{-k}(x) &= \frac{1}{2ik} e^{2\pi i k x} + \frac{1}{-2ik} e^{-2\pi i k x} \\
&= \frac{1}{k} \frac{1}{2i} \left(e^{2\pi i k x} - e^{-2\pi i k x} \right) \\
&= \frac{1}{k} \sin(2\pi k x) \; .
\end{aligned}$$

The $k = 0$ term is $\frac{1}{2}$ as before. Thus, the Fourier sine and cosine representation involves the constant term, which may be considered to be a cosine term, and a sum of sine terms corresponding to odd and positive k

$$u(x) = \frac{1}{2} + \sum_{j=0}^{\infty} \frac{1}{2j+1} \sin(2\pi(2j+1)x) \; .$$

You can get a feel for Fourier series by looking at approximations using the first few terms. If you take just the constant term, you get the "approximation"

$$u(x) \approx \frac{1}{2} \ .$$

This "approximates" the step function by its mean value. If you keep the $j = 0$, $k = 1$, sine term, the approximation is

$$u(x) \approx \frac{1}{2} + \sin(2\pi x) \ .$$

This approximation has more in common with the step function in that it is larger when $x < \frac{1}{2}$ where $u(x) = 1$ and smaller when $x > \frac{1}{2}$. It has *overshoot*, in that the maximum of the approximation is $\frac{3}{2}$ (at $x = \frac{1}{4}$). Including the $j = 1$, $k = 3$, term gives the better approximation

$$u(x) \approx \frac{1}{2} + \sin(2\pi x) + \frac{1}{3}\sin(6\pi x) \ .$$

The extra term lowers the overshoot at $x = \frac{1}{4}$ from $\frac{3}{2}$ to $\frac{7}{6}$.

Efficiency of the Fourier series representation

An infinite sum representation such as (18) is *efficient* if you get an accurate approximation with a small number of terms. We just saw that the Fourier expansion of the step function is not very efficient. Keeping just three terms gives a poor approximation to the step function. We will see that with $u(x)$ is *smooth* then the Fourier series expansion is efficient. How efficient depends on the degree of smoothness. The efficiency come s from the fact that Fourier coefficients (19) of a smooth function go to zero rapidly as $|k| \to \infty$. How rapidly depends on the degree of smoothness. The step function is not smooth and its Fourier coefficients go to zero slowly.

In Fourier analysis, saying u is *smooth* means that it has some bounded derivatives. The more derivatives are bounded, the smoother the function. The relation between bounded derivatives and decay of Fourier coefficients can be seen using integration by parts and the differentiation formula (17). For example, u has one bounded derivative means that there is a bound, M, so that

$$\left| \frac{d}{dx} u(x) \right| \leq M \ , \ \text{ for all } x \ .$$

In this case, the Fourier coefficients of u with $k \neq 0$ have

$$\begin{aligned} a_k &= \int_0^1 e^{-2\pi i k x}\, u(x)\, dx \\ &= \frac{1}{-2\pi i k} \int_0^1 \left(\frac{d}{dx} e^{-2\pi i k x} \right) u(x)\, dx \\ &= \frac{1}{2\pi i k} \int_0^1 e^{-2\pi i k x} \frac{d}{dx} u(x)\, dx \end{aligned}$$

The boundary terms in integration by parts cancel because the integrand is periodic. This leads to the ineqality

$$|a_k| \leq \frac{1}{2\pi\,|k|} M \ .$$

To see this,

$$\left| \int_0^1 e^{-2\pi ikx} \frac{d}{dx} u(x)\, dx \right| \leq \int_0^1 \left| e^{-2\pi ikx} \frac{d}{dx} u(x) \right| \, dx = \int_0^1 \left| \frac{d}{dx} u(x) \right| \, dx = M \ .$$

You can repeat this argument using more derivatives. Suppose u has n bounded derivatives and

$$\left| \frac{d^n}{dx^n} u(x) \right| \leq M \ , \quad \text{for all } x \ .$$

Then

$$|a_k| \leq \frac{M}{(2\pi\,|k|)^n} \ . \tag{21}$$

Larger n is what we mean by "more smoothness". Larger n in (21) implies that a_k decays to zero faster.

You will notice that the bound (21) is not *sharp* in the sense that a_k may go to zero faster than the bound requires. For example, this reasoning applied to the step function example (with no smoothness) would not suggest even that $a_k \to 0$ as $|k| \to \infty$. Issues like this in Fourier analysis can be deep and technical.

How is decay of Fourier coefficients related to efficiency? Write $u_N(x)$ for the partial sum of the Fourier series with terms up to $|k| = N$.

$$u_N(x) = \sum_{k=-N}^{k=N} a_k e^{2\pi ikx} \ .$$

Let $v_N(x)$ be the remainder

$$v_N(x) = u(x) - u_N(x) = \sum_{|k|>NN} a_k e^{2\pi ikx} \ .$$

Then $u \approx u_N$ if v_N is small. A inequality related to this is that uses the smoothness coefficient bound (21) is

$$\begin{aligned} |v_n(x)| &\leq 2 \sum_{k=N+1}^{\infty} \frac{M}{(2\pi|k|)^n} \\ &\leq \frac{2M}{(2\pi)^n} \int_N^\infty s^{-n}\, ds \\ |v_n(x)| &\leq \frac{2M}{(2\pi)^n(n-1)} \frac{1}{N^{n-1}} \end{aligned}$$

The complicated constant on the right is not so important, especially because the inequalities are not sharp. The important thing is that the power of N gets better (faster decay to zero) as the degree of smoothness, n, increases.

We just saw that if a function is smooth then its Fourier coefficients decay rapidly. This goes both ways. If the Fourier coefficients decay rapidly then the function is smooth. You can differentiate the Fourier series representation(18) term by term to get the Fourier series representation of the derivative:

$$\frac{d}{dx}u(x) = \sum_{k=-\infty}^{\infty} 2\pi i k a_k e^{2\pi i k x} \ . \tag{22}$$

This shows that the Fourier coefficients of $\frac{d}{dx}u$ are found by multiplying the Fourier coefficients of u by the *symbol*, $2\pi ik$. If the Fourier coefficients of u decay like a power of k, then the coefficients of $\frac{d}{dx}u$ decay like a power, one less, since

$$|a_k| \leq C\,|k|^{-n} \implies |2\pi i k a_k| \leq C'\,|k|^{-(n-1)}$$

The Fourier coefficients of the derivative still decay rapidly, but not as rapidly.

Period and wave number

Suppose u is periodic with period $L \neq 1$. The corresponding Fourier series representation involves basis functions (6). We use the inner product (10) for period L. The orthogonality relation for these basis function in this inner product are

$$\langle e_j, e_k \rangle = L\delta_{jk} \ .$$

A period L Fourier series representation (5) for u may be written out explicitly as

$$u(x) = \sum_{k=-\infty}^{\infty} a_k e^{2\pi i k x/L} \ .$$

The orthogonality relations give formulas for the coefficients:

$$\begin{aligned} \langle e_j, u \rangle &= L a_j \\ a_j &= \frac{1}{L}\int_0^L e^{-2\pi i k x/L} u(x)\, dx \ . \end{aligned}$$

Fourier analysis is used to understand differentiation and differential equations, which is the reason this Crash Course on PDE" starts with Fourier analysis. The differentiation formulas for Fourier modes, as you can see in (17) are simple when expressed in terms of p, which is the *wave number*. The Fourier mode e_k, see (6), has wave number

$$p_k = \frac{2\pi k}{L} \ .$$

The wave number is an eigenvalue of the "differentiation operator" in the sense that

$$\frac{d}{dx} e_k = p_k e_k \ . \tag{23}$$

The *wavelength* of e_k is its period, which is the smallest number L_k so that $e_k(x + L_k) = e_k(x)$. Plug into (6), and you see

$$L_k = \frac{L}{k} = \frac{2\pi}{p_k} \ .$$

A "long wave" has L_k large and p_k small. A large wave number wave is the opposite: large p and small L.

Much PDE intuition is expressed in terms of wave number and wavelength. For example, in the heat equation large wave number modes decay quickly (explanations in the next session). This implies that the solution has mostly small wave number modes, which have small derivatives. The overall solution, which is a Fourier sum of the modes that have not decayed away, has a derivative that is not large, and definitely no discontinuities.

More subtle is systems that are *dispersive*. This means, roughly, that waves with different wave number move at different speeds. Roughly speaking, many modes much be at the same place to add up to a clean discontinuity. If different modes move at different speeds, the discontinuity can break up into a sequence of oscillations with different wave numbers. This happens in physical systems such as water waves. It also happens in numerical systems that approximate PDEs. An *advection equation* is a kind of PDE that preserves discontinuities. But some numerical approximations have dispersion that causes the discontinuity in the numerical solution to break apart into a sequence of waves.

The gap between neighboring wave numbers is (because $p_{k+1} - p_k = p_1 - p_0 = p_1$)

$$\Delta p = p_{k+1} - p_k = \frac{2\pi}{L} \ . \tag{24}$$

The wave numbers are more closely spaced when the interval, L, is larger. In the limit $L \to \infty$ the gap between wave numbers goes to zero and the Fourier sum converges to the *Fourier integral*. You can give an informal derivation of the Fourier integral formulas from the Fourier series formulas using a scaling change of variables. Suppose $u(x)$ is not periodic but goes to zero as $|x| \to \infty$ (think of $u(x) = e^{-x^2}$). Replace this by a periodic function $u_L(x)$ with period L by taking $u_L(x) = u(x)$ if $|x| \leq \frac{l}{2}$. Then define $u_L(x)$ "by periodicity", just repeating $u_L(x)$ over each period of length L. If $|x| < \frac{L}{2}$, the Fourier series formula for the periodic function u_L apply to u as well. The dependence on L is included because L will be changing.

$$u(x) = \sum_{k=-\infty}^{\infty} a_k(L) e^{2\pi i k x / L} \tag{25}$$

$$a_k(L) = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{-2\pi i k x / L} u(x) \, dx \ . \tag{26}$$

We define a re-scaled Fourier coefficient written in terms of the wave number p_k rather than the mode number k:

$$\widehat{u}_L(p_k) = La_k(L) = \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{-ip_k x} u(x)\, dx \; .$$

The factor of L is so that the $L \to \infty$ limit exists. In the limit, p can be any real number and the integration domain is the whole real axis. The resulting $\widehat{u}(p)$ is the *Fourier transform* of u.

$$\widehat{u}(p) = \lim_{L\to\infty} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{-ipx} u(x)\, dx = \int_{-\infty}^{\infty} e^{-ipx} u(x)\, dx \; . \tag{27}$$

We re-write the Fourier series (25) in terms of $\widehat{u}_L(p_k)$ as

$$u(x) = \frac{1}{L} \sum_{k=-\infty}^{\infty} \widehat{u}_L(p_k)\, e^{ip_k x} \; .$$

This is exactly equivalent to (25) and it holds only for $|x| < \frac{L}{2}$. The range of validity grows to become all x in the limit $L \to \infty$. Next, write $\frac{1}{L}$ in terms of Δp using (24). This gives

$$u(x) = \frac{1}{2\pi} \left[\Delta p \sum_{k=-\infty}^{\infty} \widehat{u}_L(p_k)\, e^{ip_k x} \right] \tag{28}$$

The quantity in square brackets $[\cdots]$ is Δp trapezoid rule approximation to the integral. The limit $L \to \infty$ is equivalent to $\Delta p \to 0$, so

$$\lim_{\Delta p \to 0} \; \Delta p \sum_{k=-\infty}^{\infty} \widehat{u}_L(p_k)\, e^{ip_k x} = \int_{p=-\infty}^{\infty} \widehat{u}(p)\, e^{ipx}\, dp \; .$$

The $L \to \infty$ and $\Delta p \to 0$ limit of the Fourier series formula (28) is called the *Fourier inversion* formula.

$$u(x) = \frac{1}{2\pi} \int_{p=-\infty}^{\infty} \widehat{u}(p)\, e^{ipx}\, dp \; . \tag{29}$$

Bullet points:

- The Fourier inversion formula represents a general function u as an integral of complex exponentials e^{ipx} with coefficients $\widehat{u}(p)$. This is analogous to the Fourier series representation (18) for periodic functions.
- The sum (18) goes to an integral in the $L \to \infty$ limit because $\Delta p \to 0$, which means that all wave numbers are allowed when the interval is infinite while the $L < \infty$ case uses only the discrete set of wave numbers $p_k = k\Delta p$.
- The integral that defines the Fourier coefficients in the finite L case, re-scaled by a factor of L, converges to the Fourier transform integral (27).
- The formula that represents u in terms of $\widehat{u}$ "inverts" the Fourier transform integral (27), so it is called the *inversion* formula.

Conventions

There are many versions the Fourier series and Fourier transform formulas. Much of the diversity involves the 2π factors. For example, you can define the Fourier transform and Fourier inversion formula pairs as

$$\begin{aligned}
\widehat{u}(p) &= \frac{1}{2\pi}\int e^{-ipx}u(x)dx \\
u(x) &= \int e^{ipx}\widehat{u}(dp)dp \\
&\text{or} \\
\widehat{u}(p) &= \int e^{-2\pi ipx}u(x)dx \\
u(x) &= \int e^{2\pi ipx}\widehat{u}(dp)dp \\
&\text{or} \\
&\vdots
\end{aligned}$$