3. Lectures 13, 14: Time series analysis

Plan :

- ◇ Fourier series and transform
- ◇ Discrete Fourier transform and FFT

3.1. **Motivation for Fourier series.** Consider an example that goes back to the original work of Fourier – the heat equation.

Example. We are asked to find the temperature distribution in a thin rod of length L, insulated from the sides so that the heat flows only along the direction of the rod, and with fixed temperature at the ends. If T is absolute temperature, ρ is density, c is the heat capacity then the energy balance is given by

$$\rho c T_t + q_x = 0,$$

where q is the heat flux function. Assuming that

$$q = -\lambda T_x$$

according to Fourier, where λ is the heat conduction coefficient, we obtain

$$\rho c T_t = (\lambda T_x)_x \,.$$

The boundary conditions at $x = 0$ and $x = L$ are $T(0,t) = T(L,t) = T_0$. Now assuming that ρ, c, and λ are constants and defining $u = (T - T_0)/T_0$, $\kappa = \lambda/\rho c$, we obtain

$$u_t = \kappa u_{xx}, \quad x \in (0, L)\,, t > 0 \tag{3.1}$$

with boundary and initial conditions

$$u(0,t) = 0, \quad u(L,t) = 0 \tag{3.2}$$

and

$$u(x,0) = f(x)\,. \tag{3.3}$$

Solution. How do we solve this problem?

Here is the main idea. We look for a solution that is separable as $u = T(t)\,X(x)$ (why this makes sense will be explained at the end). Then, putting this into (3.1) we find $T_t X = \kappa T X''$ and dividing this equation by $\kappa T X$, we find

$$\frac{T_t}{\kappa T} = \frac{X''}{X}.$$

Here the left hand side depends only on t, the right-hand side only on x, hence they must be both equal to the same constant, call it $-\mu^2$:

$$\frac{T_t}{\kappa T} = \frac{X''}{X} = -\mu^2.$$

We will show that this separation constant must indeed be negative. For that look at the x-problem, $X'' = -\mu^2 X$, multiply it by X and integrate over $(0, L)$:

$$\int_0^L X X'' dx = -\mu^2 \int_0^L X^2 dx.$$

Integrate the left-hand side by parts $\int_0^L XX''dx = XX'|_0^L - \int_0^L (X')^2\, dx = -\int_0^L (X')^2\, dx$. Therefore

$$-\int_0^L \left(X'\right)^2 dx = -\mu^2 \int_0^L X^2 dx$$

$$\mu^2 = \frac{\int_0^L (X')^2\, dx}{\int_0^L X^2 dx} > 0.$$

Note that μ cannot be zero, since then X would have to be 0, which is not what we want.

Now we have the e-value problem for X:

$$X'' + \mu^2 X = 0$$
$$X(0) = X(L) = 0.$$

This is solved by

$$X_n = \sin(\mu_n x), \quad \mu_n = \frac{n\pi}{L}, \quad n = 1, 2, ...$$

Knowing μ_n, we can also solve the time part

$$T' = -\kappa\mu_n^2 T,$$

which is solved by

$$T_n = e^{-\kappa\mu_n^2 t}.$$

Now we end up with infinitely many particular solutions of the PDE subject to the homogeneous boundary conditions

$$u_n(x,t) = T_n(t)\, X_n(x) = e^{-\kappa\mu_n^2 t}\sin(\mu_n x).$$

Will any superposition of them

$$u = \sum_{n=1}^{\infty} b_n e^{-\kappa\mu_n^2 t}\sin(\mu_n x)$$

also solve the problem? Here is where we face some questions coming up because we are dealing with infinite series that may or may not converge, that may or may not be differentiable, etc.

Looking at this example with the linear algebra glasses on, we interpret the previous calculation as follows.

Let

$$u = \sum_{n=1}^{\infty} u_n(t)\, \phi_n(x) \tag{3.4}$$

where $u_n = b_n \exp\left(-\kappa\mu_n^2 t\right)$ and $\phi_n(x) = \sin\mu_n x$. Now notice that (3.4) looks exactly like a vector expanded in a certain basis: $\mathbf{u} = \sum_{k=1}^n u_k \mathbf{e}_k$, except now we have functions instead of vectors, and we have infinitely many terms in (3.4).

To expand on the analogy, suppose we need to solve the linear system $A\mathbf{x} = \mathbf{b}$ where A is $n\times n$ and nonsingular. Suppose e-vectors of A form a basis for $\mathbb{R}^n$. Let $\mathbf{e}_k$ be those e-vectors, $A\mathbf{e}_k = \lambda_k\mathbf{e}_k$. Expand the solution vector $\mathbf{x}$ in that basis: $\mathbf{x} = \sum x_k\mathbf{e}_k$. Then

$$A\sum x_k\mathbf{e}_k = \sum x_k A\mathbf{e}_k = \sum x_k\lambda_k\mathbf{e}_k = \mathbf{b}.$$

The last equation is an expansion of $\mathbf{b}$ in the basis of $\mathbf{e}_k$, hence

$$x_k = \frac{\mathbf{b}\cdot\mathbf{e}_k}{\lambda_k\|\mathbf{e}_k\|^2}$$

gives the components of the solution vector $\mathbf{x}$, and so we have the answer.

By analogy, we could have reasoned on the heat equation problem as follows. Rewrite the problem as

$$\begin{aligned} \hat{L}u &= -\frac{1}{\kappa}u_t \\ u &= 0 \text{ at } x = 0, L \\ u &= f(x) \text{ at } t = 0 \end{aligned}$$

where $\hat{L}$ is the operator $-\partial^2/\partial x^2$. Now suppose $\hat{L}$ with the above homogeneous boundary conditions has e-functions $\phi_n(x)$, and we know they are $\phi_n = \sin\left(\frac{n\pi x}{L}\right)$. The e-values are $\lambda_k = (n\pi/L)^2$. Assuming ϕ_n form a basis for the function space in which our solution u lives, we expand it in the basis as

$$u(x,t) = \sum_{k=0}^{\infty} u_k(t)\,\phi_k(x)$$

and substitute this expansion into the PDE:

$$\hat{L}u = \hat{L}\sum_{k=0}^{\infty} u_k(t)\,\phi_k(x) = \sum_{k=0}^{\infty} u_k(t)\,\hat{L}\phi_k(x) = \sum_{k=0}^{\infty} u_k(t)\,\lambda_k\phi_k(x) = -\frac{1}{\kappa}\sum_{k=0}^{\infty}\frac{du_k(t)}{dt}\phi_k(x).$$

From here

$$\frac{du_k}{dt} = -\kappa\lambda_k u_k,$$

which is solved by

$$u_k = b_k e^{-\kappa\lambda_k t}.$$

We end up with the same solution as before, with b_k found from the initial condition.

So, the bottom line is that the method of separation of variables by assuming $u = T(t)\,X(x)$ is essentially searching for components of the solution in a basis made of $X's$, and the basis is that of the the eigenfunctions of the spatial derivative operator ∂_{xx}.

The functions ϕ_n above are orthogonal in the sense that

$$(\phi_n(x), \phi_m(x)) = \int_0^L \phi_n(x)\,\phi_m(x)\,dx = \begin{cases} 0, & n \neq m \\ \|\phi_n\|^2, & n = m. \end{cases}$$

The norm of the above functions can be found as

$$\|\phi_n\|^2 = \int_0^L \left(\sin\frac{n\pi x}{L}\right)^2 dx = \frac{L}{2}.$$

Then the coefficients of the expansion are

$$u_n(t) = \frac{2}{L}\int_0^L u(x,t)\,\phi_n(x)\,dx.$$

Using the initial condition $u(x,0) = f(x)$, we find that

$$b_n = \frac{2}{L}\int_0^L f(x)\,\phi_n(x)\,dx.$$

This gives us the complete solution of the heat equation problem:

$$\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} b_n e^{-\kappa\mu_n^2 t}\sin(\mu_n x), \\ b_n &= \frac{2}{L}\int_0^L f(x)\sin(\mu_n x)\,dx, \\ \mu_n &= \frac{n\pi}{L}. \end{aligned}$$

3.2. **Fourier series.** Now we give some formal results justifying the steps used above to arrive at the final solution.

The main question is:

- ⋄ Given any integrable function $f(x)$ on $x \in (-L, L)$ and the series

$$FS(f) = \frac{a_0}{2} + \sum_{k=1}^{\infty}\left(a_k \cos\frac{\pi k x}{L} + b_k \sin\frac{\pi k x}{L}\right)$$

with

$$\begin{aligned} a_k &= \frac{1}{L}\int_{-L}^{L} f(x)\cos kx dx, \\ b_k &= \frac{1}{L}\int_{-L}^{L} f(x)\sin kx dx, \end{aligned}$$

what is the relationship between $FS(f)$ and $f(x)$?

In particular:

- ⋄ Is $FS(f) = f(x)$?
- ⋄ Can we differentiate the FS term by term?
- ⋄ Can we integrate the FS?

Most answers are positive, however, there will be some restrictions on $f(x)$.

Next we state some of the main definitions and theorems, and then we show typical examples demonstrating main properties of the Fourier series.

Definition 14. Functions $\phi_n(x)$, $n = 1, 2, ...$ are said to be *orthogonal* over $x \in [a, b]$ if

$$\int_a^b \phi_n(x)\phi_m(x)\,dx = \begin{cases} 0, & n \neq m \\ \|\phi_n\|^2, & n = m. \end{cases}$$

The nonzero quantity $\|\phi_n\| = \sqrt{\int_a^b \phi_n^2(x)\,dx}$ is the *L_2-norm* of ϕ_n. If $\|\phi_n\| = 1$, the set is *orthonormal.*

For example, the set 1, $\cos x$, $\sin x$, $\cos 2x$, $\sin 2x$, etc. is orthogonal over $[-\pi, \pi]$ and $\|1\| = \sqrt{2\pi}$, $\|\cos nx\| = \|\sin nx\| = \sqrt{\pi}$ for $n \geq 1$.

Definition 15. The series $\sum f_n(x)$ converges to $f(x)$ *pointwise* in (a, b) if for any $x \in (a, b)$

$$\lim_{n\to\infty}\left|f(x) - \sum_{k=1}^{n} f_k(x)\right| = 0.$$

Definition 16. The series $\sum f_n(x)$ converges to $f(x)$ *uniformly* in (a,b) if

$$\max_{x\in(a,b)}\left|f(x)-\sum_{k=1}^{n} f_k(x)\right| \to 0 \text{ as } n\to\infty.$$

Definition 17. The series $\sum f_n(x)$ converges to $f(x)$ in L_2 norm, if

$$\int_a^b \left|f(x)-\sum_{k=1}^{n} f_k(x)\right|^2 dx \to 0 \text{ as } n\to\infty.$$

Definition 18. Function $f(x)$ is *piecewise continuous* in $[a,b]$ if it is continuous in a finite number of subintervals of $[a,b]$ and at the boundaries of the intervals it has jump discontinuities (i.e. one-side limits exist at the jumps).

Definition 19. Function $f(x)$ is *piecewise smooth* in $[a,b]$ if both f and f' are piecewise continuous in in $[a,b]$.

Definition 20. The function

$$T_n(x)=\frac{\alpha_0}{2}+\sum_{k=1}^{n}\alpha_k\cos kx+\beta_k\sin kx$$

is called a trigonometric polynomial of order n.

Theorem 21. *The best L_2 approximation in terms of trigonometric polynomials to a square-integrable function $f(x)$ on $[-\pi,\pi]$ is provided by the partial sum of the Fourier series of f, i.e. by*

$$S_n(x)=\frac{a_0}{2}+\sum_{k=1}^{n}a_k\cos kx+b_k\sin kx,$$

where

$$\begin{aligned} a_k &= \tfrac{1}{\pi}\textstyle\int_{-\pi}^{\pi} f(x)\cos kx\,dx \\ b_k &= \tfrac{1}{\pi}\textstyle\int_{-\pi}^{\pi} f(x)\sin kx\,dx \end{aligned}.$$

Proof. This is proved by looking at the error $E=\int_{-\pi}^{\pi}\left(f(x)-T_n(x)\right)^2 dx$ and setting the derivatives of E with respect to α_k and β_k to zero. They will be zero provided that α_k and β_k are precisely the Fourier coefficients. One should also verify that the second derivative matrix is positive definite. □

From the fact that $E>0$, one can deduce the following *Bessel's inequality* for any square-integrable $f(x)$:

$$\int_{-\pi}^{\pi} f^2 dx \geq \pi\left[\frac{a_0^2}{2}+\sum_{k=1}^{n}\left(a_k^2+b_k^2\right)\right].$$

If in addition the function is 2π periodic and continuous, then the following *Parseval's equality* holds

$$\int_{-\pi}^{\pi} f^2 dx = \pi\left[\frac{a_0^2}{2}+\sum_{k=1}^{\infty}\left(a_k^2+b_k^2\right)\right].$$

The following *Weierstrass approximation theorem* holds:

Theorem 22. *For any $\epsilon > 0$ and any 2π-periodic continuous $f(x)$, there exists a trigonometric polynomial $T(x)$ such that $|f(x) - T(x)| < \epsilon$ at all x.*

That is, one can approximate any function of this type by a trigonometric polynomial with any desired accuracy.

As a consequence of the previous theorem one has the following fact.

Theorem 23. *For 2π-periodic continuous $f(x)$ the $FS(f)$ converges to f in the L_2 sense, i.e. $\|f - S_n\|_2 = \sqrt{\int_{-\pi}^{\pi} (f - S_n)^2 \, dx} \to 0$ as $n \to \infty$.*

The following lemma is useful.

Theorem 24. *Riemann-Lebesgue Lemma. Let $g(x)$ be continuous on $[a, b]$ except for a finite number of points of jump discontinuities and $\int_a^b |g(x)| \, dx < \infty$. Then*

$$\lim_{\lambda \to \infty} \int_a^b g(x) \, e^{i\lambda x} dx = 0.$$

Let $f(x)$ be 2π periodic and absolutely integrable. Then

$$\begin{aligned}
S_n(x) &= \frac{a_0}{2} + \sum_{k=1}^{n} a_k \cos kx + a_k \sin kx \\
&= \frac{1}{\pi} \int_{-\pi}^{\pi} \left[\frac{1}{2} + \sum_{k=1}^{n} (\cos kt \cos kx + \sin kt \sin kx) \right] f(t) \, dt \\
&= \frac{1}{\pi} \int_{-\pi}^{\pi} \left[\frac{1}{2} + \sum_{k=1}^{n} \cos k(t - x) \right] f(t) \, dt = \\
&= \frac{1}{\pi} \int_{-\pi}^{\pi} D_n(t - x) \, f(t) \, dt,
\end{aligned}$$

where

$$D_n(\xi) = \frac{\sin(n + 1/2)\,\xi}{2 \sin \frac{\xi}{2}}$$

is the *Dirichlet kernel.*

Due to periodicity, one can also write

$$S_n(x) = \frac{1}{\pi} \int_{-\pi}^{\pi} D_n(\xi) \, f(\xi + x) \, d\xi.$$

Now note that

$$S_n(x) - f(x) = \frac{1}{\pi} \int_{-\pi}^{\pi} D_n(\xi) \left[f(\xi + x) - f(x) \right] d\xi,$$

and the main question is:

Will this difference tend to 0 as $n \to \infty$?

The positive answer is given by the main theorem due to Dirichlet:

Theorem 25. *Dirichlet Theorem. A 2π-periodic piece-wise smooth function $f(x)$ has a Fourier series converging to $\frac{1}{2}\left[f(x_+) + f(x_-)\right]$. If $f(x)$ is continuous at all x the Fourier series converges to $f(x)$ absolutely and uniformly at all x.*

The proof is based on the above representation of $S_n(x) - f(x)$ in terms of the Dirichlet kernel and the use of the Riemann-Lebesgue lemma.

For integrability of the Fourier series one requires that the series converge uniformly. Differentiation, on the other hand, requires that the formally differentiated series converge uniformly. Precise formulations can be found elsewhere.

There is a very important property of the Fourier series of discontinuous functions that is called the Gibbs phenomenon. Basically, at a discontinuity any finite-term approximation of the Fourier series will show oscillations, the amplitude of which does not diminish with the number of terms.

For $f(x) = x$ on $(-\pi, \pi)$, the Fourier series is given by

$$f = 2\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \sin kx.$$

Consider the partial sum $S_n(x) = 2\sum_{k=1}^{n} \frac{(-1)^{k+1}}{k} \sin kx$ and look for the maximum of $S_n(x)$ at x near π_-. Let $x = \pi - \delta$ with δ small and find where $S_n'(x) = 0$. One can show that the maximum occurs at $x \approx \pi - \frac{\pi}{n}$ and the value of S_n at that point tends to

$$2\int_0^{\pi} \frac{\sin x}{x} dx \approx \pi \cdot 1.18.$$

That is the overshoot is 18% of the true maximum of π, or 9% of the total jump of 2π.

Example 26. A square pulse, triangular pulse, and sawtooth function:

$$f_1 = \begin{cases} -1, & -\pi < x < 0 \\ 1, & 0 < x < \pi \end{cases}$$
$$f_2 = |x|, \quad x \in (-\pi, \pi)$$
$$f_3 = x, \quad x \in (-\pi, \pi)$$

The Fourier series for these functions are given by

$$f_1 = \frac{2}{\pi}\sum_{k=1}^{\infty} \frac{\left[1 - (-1)^k\right]}{k} \sin kx$$
$$f_2 = \frac{\pi}{2} - \frac{2}{\pi}\sum_{k=1}^{\infty} \frac{\left[1 - (-1)^k\right]}{k^2} \cos kx$$
$$f_3 = 2\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \sin kx$$

One can represent the Fourier series in complex form using the Euler formulas for sine and cosine

$$\cos\alpha = \frac{e^{i\alpha} + e^{-i\alpha}}{2}, \quad \sin\alpha = \frac{e^{i\alpha} - e^{-i\alpha}}{2i}.$$

Then

$$FS(f) = \sum_{k=-\infty}^{\infty} c_k e^{i\frac{k\pi x}{L}}$$

where

$$c_k = \frac{1}{2L} \int_{-L}^{L} f(x)\, e^{-i\frac{k\pi x}{L}} dx.$$

This form will be useful for both deriving the Fourier transform by taking $L \to \infty$ and for introducing the Discrete Fourier transform.

3.3. **Fourier transform.** We begin with the Fourier series in complex form:

$$f_L = \sum_{k=-\infty}^{\infty} c_k e^{i\frac{k\pi x}{L}}$$

where

$$c_k = \frac{1}{2L} \int_{-L}^{L} f_L(x)\, e^{-i\frac{k\pi x}{L}} dx,$$

and let $L \to \infty$. For this, combine the previous expressions as

$$f_L = \sum_{k=-\infty}^{\infty} \frac{1}{2L} \int_{-L}^{L} f_L(u)\, e^{i\frac{k\pi(u-x)}{L}} du.$$

Now let

$$\Delta\omega = \frac{\pi}{L}, \quad \omega_k = \frac{k\pi}{L},$$

then

$$f_L = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \Delta\omega e^{-i\omega_k x} \int_{-L}^{L} f_L(u)\, e^{i\omega_k u} du.$$

As $L \to \infty$, we obtain $f_L \to f(x)$ and

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega x} \hat{f}(\omega) \tag{3.5}$$

where

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} du e^{i\omega u} f(u)\, du. \tag{3.6}$$

These define the Fourier transform pair:

$$\hat{f}(\omega) = \mathcal{F}(f),$$
$$f(x) = \mathcal{F}^{-1}\left(\hat{f}\right).$$

Basic properties of the FT are:

(1) Linearity:

$$\mathcal{F}[f+g] = \mathcal{F}[f] + \mathcal{F}[g]$$

(2) Shift:

$$\mathcal{F}[f(x-a)] = e^{i\omega a}\mathcal{F}[f(x)]$$

(3) Derivative:

$$\mathcal{F}\left[f'\right] = -i\omega\mathcal{F}[f]$$

(4) Convolution:

$$\mathcal{F}[f * g] = \mathcal{F}[f]\,\mathcal{F}[g]$$

(5) Parseval:

$$2\pi \int_{-\infty}^{\infty} |f|^2 \, dx = \int_{-\infty}^{\infty} \left|\hat{f}\right|^2 d\omega$$

Here

$$f * g = \int_{-\infty}^{\infty} f(x-y)\, g(y)\, dy$$

is the convolution of two functions $f(x)$ and $g(x)$.

Example 27. Some examples of FT are:

$$f(x) = e^{-a|x|}, \quad a > 0$$
$$\hat{f}(\omega) = \frac{2a}{a^2 + \omega^2}$$

and

$$f(x) = e^{-ax^2}, \quad a > 0$$
$$\hat{f}(\omega) = \int_{-\infty}^{\infty} e^{i\omega x} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} e^{-\omega^2/4a}.$$

This follows from $\hat{f}' = -\frac{\omega}{2a}\hat{f}$, hence $\hat{f} = ce^{-\omega^2/4a}$ and $\hat{f}(0) = \sqrt{\pi/a}$.

We see that in both cases the wide signal has a narrow inverse and vice versa.

Example 28. To illustrate the use of FT to solve PDE problems on infinite domains, consider again the heat equation

$$u_t = a u_{xx}, \quad x \in \mathbb{R}, t > 0$$

with the initial condition

$$u(x, 0) = f(x).$$

If we define the FT of $u(x,t)$ as $\hat{u}(t) = \mathcal{F}[u(x,t)]$, then

$$\hat{u}_t = \mathcal{F}[u_t(x,t)] = a\mathcal{F}[u_{xx}(x,t)] = a(-i\omega)^2 \mathcal{F}[u(x,t)] = -a\omega^2 \hat{u},$$

which is solved by

$$\hat{u} = ce^{-a\omega^2 t}.$$

The constant c can be found using the transform of the initial condition

$$\hat{f}(\omega) = \mathcal{F}[f(x)] = \mathcal{F}[u(x,0)] = \hat{u}(0) = c.$$

Then

$$\hat{u} = \hat{f}(\omega)\, e^{-a\omega^2 t}.$$

Now notice that this is a product of two transforms, therefore it is the transform of the convolution of inverse transforms of each of the multiples. Since

$$\mathcal{F}^{-1}\left[e^{-a\omega^2 t}\right] = \frac{1}{\sqrt{4\pi a t}} e^{-\frac{x^2}{4at}} = g(x,t)$$

is the *heat kernel* and $\mathcal{F}^{-1}\left[\hat{f}\right] = f(x)$, we find the final solution as

$$\begin{aligned} u(x,t) &= \int_{-\infty}^{\infty} f(y)\, g(x-y,t)\, dy \\ &= \int_{-\infty}^{\infty} f(y)\, \frac{1}{\sqrt{4\pi a t}} e^{-\frac{(x-y)^2}{4at}} dy. \end{aligned}$$

The function

$$g = \frac{1}{\sqrt{4\pi a t}} e^{-\frac{x^2}{4at}}$$

is also known as the *Green's function* of the 1D heat equation.

One can apply the FT or some variations of it to other linear problems in PDE on infinite or semi-infinite domains.

3.4. **Discrete Fourier transform and FFT.** Now we want to apply the previous ideas to transforming a finite signal to its frequency domain. We begin with a definition and then explain how it arises and is used.

The DFT of vector $f = [f_0, f_1, ..., f_{n-1}]^T$ is defined as

$$\hat{f}_k = \sum_{j=0}^{n-1} f_j e^{-2\pi i jk/n}, \tag{3.7}$$

and the inverse transform is

$$f_j = \frac{1}{n}\sum_{k=0}^{n-1} \hat{f}_k e^{2\pi i jk/n}. \tag{3.8}$$

How does one come up with this kind of a definition?

Recall the Fourier series of a function $f(x)$ on $x \in (-L, L)$,

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{i\frac{k\pi x}{L}}, \tag{3.9}$$

where

$$c_k = \frac{1}{2L}\int_0^{2L} f(x)\, e^{-i\frac{k\pi x}{L}} dx,$$

(we can shift the domain to any interval of length $2L$, say from 0 to $2L$).

Suppose now that we are not interested in all the values of $f(x)$, but only in some samples over the domain $(0, 2L)$. For example, at $x = x_j = j\Delta x$, where $j = 0, 1, 2, ..., n-1$, and $\Delta x = 2L/n$. (Note, we do not need x_n as $f_n = f_0$ by periodicity).

So we have n samples of $f(x)$ that we care about, and it is enough to have n coefficients c_k in (3.9) to uniquely identify those n samples. We can choose c_0, c_1, ..., c_{n-1} and set the rest of c_k to zero. Then s

$$f_j = f(x_j) = \sum_{k=0}^{n-1} c_k e^{i\frac{\pi k x_j}{L}} = \sum_{k=0}^{n-1} c_k e^{i\frac{2\pi k j}{n}}.$$

How do we find c_k from here? Multiply f_j by $e^{-i\frac{2\pi mj}{n}}$ and sum over all j:

$$\begin{aligned}\sum_{j=0}^{n-1} f_j e^{-i\frac{2\pi mj}{n}} &= \sum_{k=0}^{n-1}\sum_{j=0}^{n-1} c_k e^{i\frac{2\pi kj}{n}} e^{-i\frac{2\pi mj}{n}} = \\ &= \sum_{k=0}^{n-1} c_k \sum_{j=0}^{n-1} e^{i\frac{2\pi(k-m)j}{n}}. \end{aligned} \tag{3.10}$$

The inner sum here

$$\sum_{j=0}^{n-1} e^{i\frac{2\pi(k-m)j}{n}}$$

is 0 unless $k = m$, because we are adding all n-th roots of 1: e.g. when $n = 2$: $i + (-i) = 0$, $n = 3$: $1 + e^{i2\pi/3} + e^{-i2\pi/3} = 0$, $n = 4$: $1 + i - 1 - i = 0$, etc. When $k = m$, we get the sum of n ones, so it is n. Therefore, the right-hand side of (3.10) is nc_k, which gives us

$$c_m = \frac{1}{n}\sum_{j=0}^{n-1} f_j e^{-i\frac{2\pi mj}{n}}.$$

This basically explains the reasoning behind the formulas defining the discrete Fourier transform (3.7)-(3.8). The factor $1/n$ can be placed in either formula, as with the Fourier series or transform.

One more remark worth mentioning.

If in the definition of the sample

$$f_j = f(x_j) = \sum_{k=0}^{n-1} c_k e^{i\frac{\pi k x_j}{L}},$$

we go back to using any x, not just the sample point x_j, we obtain an *interpolation* formula for $f(x)$:

$$p(x) = \sum_{k=0}^{n-1} c_k e^{i\frac{\pi k x}{L}}$$

with

$$c_k = \frac{1}{n}\sum_{j=0}^{n-1} f_j e^{-i\frac{2\pi kj}{n}}$$

is a trigonometric interpolation of $f(x)$ through the samples at $x_j = j2L/n$, $j = 0, 1, 2, ..., n-1$.

Next we simplify the above expressions so that they can be written in terms matrix-vector multiplications.

Note that the complex exponentials here are all integer powers of

$$\omega = e^{-i(2\pi/n)} = e^{-i\phi}, \quad \phi = \frac{2\pi}{n}.$$

So we can write the transform pair as

$$\hat{f}_k = \sum_{j=0}^{n-1} f_j \left(\omega^k\right)^j, \quad f_j = \frac{1}{n}\sum_{k=0}^{n-1} \hat{f}_k \left(\omega^{-j}\right)^k.$$

The DFT can be written via a matrix F as

$$\hat{f} = Ff,$$

where the Fourier matrix is

$$F = \begin{bmatrix} 1 & 1 & & \dots & & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{n-2} & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \dots & \omega^{2(n-2)} & \omega^{2(n-1)} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 1 & \omega^{n-2} & \omega^{2(n-2)} & \dots & \omega^{(n-2)(n-2)} & \omega^{(n-1)(n-2)} \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \dots & \omega^{(n-1)(n-2)} & \omega^{(n-1)^2} \end{bmatrix}.$$

As for the inverse transform,

$$f = \frac{1}{n} F^* \hat{f},$$

from which we get

$$F^{-1} = \frac{1}{n} F^*,$$

or

$$FF^* = nI.$$

This is basically an orthogonality condition for F. All columns (and rows due to symmetry of F) are orthogonal to each other. The norm of each column is $\sqrt{n}$, and so $\frac{1}{\sqrt{n}}F$ is unitary.

Remark. In Matlab, the DFT of vector x to vector y is performed as

$$y_{p+1} = \sum_{j=0}^{n-1} x_{j+1} \omega^{jp},$$

where $\omega = e^{-2\pi/n}$. The commands are $y = fft\,(x)$ and $x = ifft\,(y)$.

Some examples of DFT follow.
Let us transform the following vectors

$$f_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, f_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, f_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, f_4 = \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix}.$$

The corresponding Fourier matrix is

$$F_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix}.$$

since $\omega = e^{-i\pi/2} = -i$. Hence

$$\hat{f}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \hat{f}_2 = \begin{bmatrix} 1 \\ -i \\ -1 \\ i \end{bmatrix}, \hat{f}_3 = \begin{bmatrix} 4 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \hat{f}_4 = \begin{bmatrix} 0 \\ 0 \\ 4 \\ 0 \end{bmatrix}.$$

3.5. **FFT.** The key thing to note here is that since $\omega = e^{-i\phi}$ is the n-th root of 1, then there are only n distinct values of ω. Yet, matrix F contains about $n-2$ more values of powers of ω, hence there is redundancy in the matrix. Generally, an $n \times n$ matrix will need n^2 multiplications with a vector to produce another vector. Here, we see that there are only about n distinct number in Ff. So there is a chance to save big time on multiplication. The problem is to arrange those distinct numbers in F so that Ff is found in as few multiplications as possible.

Consider some examples with small n to get an idea.

Example 29. Fourier matrix for $n = 4$ has $\omega = e^{-i\pi/2} = -i$, so

$$F_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{bmatrix}.$$

Now note that $\omega^4 = 1$, $\omega^6 = \omega^2$, $\omega^9 = \omega^8\omega = \omega$, hence

$$F_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & 1 & \omega^2 \\ 1 & \omega^3 & \omega^2 & \omega \end{bmatrix},$$

which contains only four distinct powers of ω: 1, ω, ω^2, ω^3 out of 16 total numbers in the matrix. Now consider

$$F_2 = \begin{bmatrix} 1 & 1 \\ 1 & \omega \end{bmatrix}$$

and notice that

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & 1 & \omega^2 \\ 1 & \omega^3 & \omega^2 & \omega \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -i \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & i \end{bmatrix}}_{\text{contains diagonal matrices}} \underbrace{\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & \omega & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & \omega \end{bmatrix}}_{\text{built from } F_2} \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{\text{even-odd permutations}}$$

Generally,

$$F_{2N} = \begin{bmatrix} I_N & D_N \\ I_N & -D_N \end{bmatrix} \begin{bmatrix} F_N & 0 \\ 0 & F_N \end{bmatrix} \begin{bmatrix} \text{even-odd} \\ \text{permutation} \end{bmatrix}$$

where D_N is diagonal with entries $\left(1, \omega, ..., \omega^{N-1}\right)$.

So when F_{2N} multiplies a vector f

$$F_{2N} f = \begin{bmatrix} I_N & D_N \\ I_N & -D_N \end{bmatrix} \begin{bmatrix} F_N & 0 \\ 0 & F_N \end{bmatrix} Pf$$

it first multiplies f with a permutation matrix to rearrange the components of f:

$$Pf = P \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ ... \\ f_{2N-1} \end{bmatrix} = \begin{bmatrix} f_0 \\ f_2 \\ f_4 \\ ... \\ f_{2N-3} \\ f_{2N-1} \end{bmatrix} = \begin{bmatrix} f_{even} \\ f_{odd} \end{bmatrix}.$$

Then

$$\begin{bmatrix} F_N & 0 \\ 0 & F_N \end{bmatrix} \begin{bmatrix} f_{even} \\ f_{odd} \end{bmatrix} = \begin{bmatrix} F_N f_{even} \\ F_N f_{odd} \end{bmatrix}$$

which is now two matrix-vector multiplications of order N. These are reduced the same way to a multiplication of order $N/2$, and so on. The overall cost of this multiplication is $\frac{1}{2}N\log_2 N$. If for example, direct multiplication for $N = 1024$ would require $N^2 = 2^{20} = 1048576$ operations, with the FFT, we get only 5120, a number 204 times smaller.

Example 30. Application of FFT to time series analysis. The power spectrum.

We look at the signal consisting of two frequencies and with some added noise. The clean part is

$$f = \sin(\omega_1 t) + \sin(\omega_2 t)$$

where $\omega_1 = 2\pi \cdot 50$ and $\omega_2 = 2\pi \cdot 120$.

This signal is sampled over $dt = 0.001$ from $t = 0$ to $t = 1$, so we have 1000 points in vector f.

If $\hat{f} = Ff$ is the Fourier transform of the signal, then the power spectrum is given by

$$p = \hat{f}. * \hat{f} = \left[\left|\hat{f}_0\right|^2, \left|\hat{f}_1\right|^2, \left|\hat{f}_2\right|^2, ..., \left|\hat{f}_{n-1}\right|^2\right]^T$$

and each component here measures how much energy is contained in the corresponding frequency.

Example 31. Application of FFT to calculate derivatives.

Given a function $f(x)$ and its transform $\hat{f}(k)$, we can relate the derivative $f'(x)$ and its transform as $\mathcal{F}[f'] = i\omega\hat{f}$. The numerical derivative is approximated by first finding the transform $\hat{f}$, then multiplying it by $i\omega$, then inverse transforming:

$$f' = \mathcal{F}^{-1}[i\omega\mathcal{F}[f(x)]] = \mathcal{F}^{-1}\left[i\omega\hat{f}\right]$$

For example, we look at

$$f = \cos x\, e^{-x^2/25},$$

and approximate its derivative by both finite difference formula

$$f' \approx \frac{f_{i+1} - f_i}{\Delta x}$$

and spectrally to see how the spectral formula performs.

Example 32. Application of FFT to solve the advection equation

For the advection equation,

$$u_t + cu_x = 0,$$

the exact solution is

$$u(x,t) = f(x - ct)$$

where $f(x)$ is the initial condition. One can transform to the Fourier space and integrate the equation for the transform

$$\hat{u}_t + i\omega\hat{u} = 0$$

once this is done, the final solution is

$$u(x,t) = \mathcal{F}^{-1}[\hat{u}(\omega,t)].$$