18.085/18.0851 Computational Mathematical Engineering I **Summer 2020**

Week 9 (August 3rd-August 7th)

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Last week we learned about the Fourier transform and the computation of some important functions, including the box function, the delta function, and the Gaussian. This lecture is dedicated to the application of the Fourier transform.

9.1 Application 1: Heat Equation

One of the very first applications of the Fourier transform is solving heat equations. In one dimension, the heat equation can be written as

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{9.1}$$

This equation governs the heat flow in one dimension. Because it is dependent on both space and time, we need to specify both the intial and boundary conditions. Often time, you would see something like

$$u(x, t = 0) = f(x) \tag{9.2}$$

$$u(x,t)|_{x\in\partial\Omega} = g(x,t) \tag{9.3}$$

For well-behaved boundary conditions, we can again use separation of variables, ie. $u(x) = X(x)T(t)$. But what about infinite boundary, ie.

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, x \in \mathbb{R} \tag{9.4}$$

$$u(x, t = 0) = f(x) \tag{9.5}$$

In that case, we would resort to Fourier transform. Assuming the solution can be written as the Fourier transform, we have

$$\hat{u}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,t) e^{-ikx} dx \tag{9.6}$$

Hence we take the heat equation and perform the Fourier transform on both sides

$$\int_{-\infty}^{\infty} \frac{\partial u(x,t)}{\partial t} e^{-ikx} dx = \alpha \int_{-\infty}^{\infty} \frac{\partial^2 u(x,t)}{\partial x^2} e^{-ikx} dx \tag{9.7}$$

Performing some algebra, we have

$$\frac{\partial}{\partial t}\left(\int_{-\infty}^{\infty} u(x,t) e^{-ikx} dx\right) = \alpha \int_{-\infty}^{\infty} \frac{\partial^2 u(x,t)}{\partial x^2} e^{-ikx} dx \tag{9.8}$$

$$\frac{\partial \hat{u}(k,t)}{\partial t} = \alpha \int_{-\infty}^{\infty} \frac{\partial^2 u(x,t)}{\partial x^2} e^{-ikx} dx \tag{9.9}$$

We shall perform the integration by parts twice on the right hand side, namely that

$$\int_{-\infty}^{\infty} \frac{\partial^2 u(x,t)}{\partial x^2} e^{-ikx} dx = \int_{-\infty}^{\infty} (-ik) \frac{\partial u(x,t)}{\partial x} e^{-ikx} dx \tag{9.10}$$
$$= \int_{-\infty}^{\infty} (-ik)^2 \frac{\partial u(x,t)}{\partial x} e^{-ikx} dx \tag{9.11}$$
$$= \int_{-\infty}^{\infty} -(k)^2 u(x,t) e^{-ikx} dx \tag{9.12}$$
$$= -(k)^2 \hat{u}(k,t) \tag{9.13}$$

Suppressing the explicit variable notation, we therefore arrived at the ordinary differential equation over t, ie.

$$\hat{u}_t = -\alpha k^2 \hat{u} \tag{9.14}$$

whose solution we know as

$$\hat{u}(k,t) = \hat{u}_0 e^{-\alpha k^2 t} \tag{9.15}$$

where $\hat{u}_0 = \hat{u}(k, t = 0)$. Hence, to get $u(x,t)$, we just have to perform the inverse Fourier transform on $\hat{u}(k,t)$, ie.

$$u(x,t) = \mathscr{F}^{-1}(\hat{u}(k,t)) \tag{9.16}$$
$$= \mathscr{F}^{-1}(\hat{u}_0 e^{-\alpha k^2 t}) \tag{9.17}$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} u_0(y) e^{-iky} dy \right) e^{-\alpha k^2 t} e^{ikx} dk \tag{9.18}$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u_0(y) e^{-\alpha k^2 t} e^{ik(x-y)} dk dy \tag{9.19}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u_0(y) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha k^2 t} e^{ik(x-y)} dk dy \tag{9.20}$$
$$\tag{9.21}$$

Note that if we define

$$h(x) = \mathscr{F}^{-1}(e^{-\alpha k^2 t}) \tag{9.22}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha k^2 t} e^{ik(x)} dk \tag{9.23}$$
$$\tag{9.24}$$

Then

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u_0(y) h(x-y) dy \tag{9.25}$$

Hence we just have to compute $h(x)$:

$$h(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha k^2 t} e^{ikx} dk \tag{9.26}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha t(k^2 - i(x/(\alpha t))k)} dk \tag{9.27}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha t(k^2 - 2(k)(ix/2) + (ix/(2\alpha t))^2 - (ix/(2\alpha t))^2)} dk \tag{9.28}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha t(k - (ix/(2(\alpha t))))^2} e^{-\alpha(x/(2(\alpha t)))^2} dk \tag{9.29}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha t(k)^2} e^{-\alpha(x/(2(\alpha t)))^2} dk \tag{9.30}$$
$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\pi}{\alpha t}} e^{-(x^2/(4\alpha t))} \tag{9.31}$$
$$= \frac{1}{\sqrt{2}} \sqrt{\frac{1}{\alpha t}} e^{-(x^2/(4\alpha t))} \tag{9.32}$$
$$\tag{9.33}$$

Hence, the solution $u(x,t)$ is

$$u(x,t) = \frac{1}{\sqrt{4\pi\alpha t}} \int_{-\infty}^{\infty} u_0(y) e^{-\frac{(x-y)^2}{4\alpha t}} dy \tag{9.34}$$

A few comments

- The exponential term in the integrand is called the heat kernel
- The heat kernel is smoothing: any choppy initial condition will be smoothened out by the heat kernel
- Heat goes from hot places to cold places. See demo.

9.2 Discrete Fourier Transform

Now we would like to turn out study to computational Fourier analysis: the discrete Fourier transform.

Here are the clarifications of the languages.

- Fourier series: a representation of periodic functions
- Fourier transform: a representation of non-periodic, rapidly decreasing functions
- Discrete Fourier transform: computational Fourier series
- Fast Fourier transform: a fast way of doing discrete Fourier series and transform
- Discrete/Fast Fourier series: same as above

We will begin with the definition of discrete Fourier transform: suppose we have an interval $[0, L]$ and we discretize into N points: $x_0, ..., x_{N-1}$. Then if the value of u at x_j is u_j, the DFT of u at that point would be

$$\hat{u}_k^d = \frac{1}{N} \sum_{k=0}^{N-1} u_j e^{-ik2\pi j/N} \tag{9.35}$$

where $k = 0, ..., N-1$.

Just like the continuous Fourier series, there is some prefactor, which is based on the orthogonality relation. We can easily check that

$$\frac{1}{N} \sum_{k=0}^{N-1} e^{il2\pi k/N} e^{-ij2\pi k/N} = \delta_{jl} \tag{9.36}$$

Here is the proof:

- If $l = j$, then the sum is equal to 1 upon dividing by N
- If $l \neq j$, then

$$\begin{aligned} \frac{1}{N} \sum_{k=0}^{N-1} u_j e^{-ik2\pi j/N} &= \frac{1}{N} \sum_{k=0}^{N-1} \left(e^{i2\pi(l-j)/N} \right)^k && (9.37) \\ &= \frac{1}{N} \frac{1 - (e^{i2\pi(l-j)/N})^N}{1 - e^{i2\pi(l-j)/N}} && (9.38) \\ &= 0 && (9.39) \end{aligned}$$

Solving for $\hat{u}_k^d$ will involve some matrix operation $Au = b$, where

$$\begin{aligned} A_{kj} &= \frac{1}{N} e^{-ik2\pi j/N} && (9.40) \\ u &= u_j && (9.41) \\ b_j &= \hat{u}_k^d && (9.42) \end{aligned}$$

9.3 Fourier series over Arbitrary Interval

Before we talk about the relation between Fourier series and discrete Fourier transform I would first like to tie up a loose end: Fourier series over any interval $[a, b]$, such that $L = b - a$.
In that case, the complex representation should use the basis $e^{i2\pi k/L}$, and the representation should be

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{i2\pi xk/L} \tag{9.43}$$

where

$$c_k = \frac{1}{L} \int_a^b f(x) e^{-ik2\pi x/L} dx \tag{9.44}$$

This is because

$$f(x)e^{-ik2\pi x/L} = \sum_{j=-\infty}^{\infty} c_j e^{i2\pi xj/L} e^{-ik2\pi x/L} \tag{9.45}$$

$$\int_a^b f(x)e^{-ik2\pi x/L}dx = \int_a^b \sum_{j=-\infty}^{\infty} c_j e^{i2\pi xj/L} e^{-ik2\pi x/L}dx \tag{9.46}$$

$$\int_a^b f(x)e^{-ik2\pi x/L}dx = \sum_{j=-\infty}^{\infty} c_j \int_a^b e^{i2\pi xj/L} e^{-ik2\pi x/L}dx \tag{9.47}$$

$$\int_a^b f(x)e^{-ik2\pi x/L}dx = \sum_{j=-\infty}^{\infty} c_j \int_a^b e^{i2\pi xj/L} e^{-ik2\pi x/L}dx \tag{9.48}$$

$$\int_a^b f(x)e^{-ik2\pi x/L}dx = c_k L \tag{9.49}$$

$$c_k = \frac{1}{L}\int_a^b f(x)e^{-ik2\pi x/L}dx \tag{9.50}$$

- When $(a, b) = (-\pi, \pi)$, $L = 2\pi$ and the basis becomes $e^{i2\pi kx/(2pi} = e^{ikx}$
- When $(a, b) = (-l, l)$, $L = 2l$ and the basis becomes $e^{i2\pi kx/(2l} = e^{ik\pi x}$
- When $(a, b) = (0, l)$, $L = l$ and the basis becomes $e^{i2\pi kx/l}$

9.4 Relations Between Fourier series and Discrete Fourier Transform

Given a function $u(x)$, we can write down its Fourier series over the interval $[0, L]$

$$u(x) = \sum_{l=-\infty}^{\infty} c_k e^{il2\pi x/L} \tag{9.51}$$

If we plug this in to the expression of the discrete Fourier transform, assuming $x_j = jL/N$

$$\hat{u}_k^d = \frac{1}{N}\sum_{k=0}^{N-1} u_j e^{-ik2\pi j/N} \tag{9.52}$$

$$= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{l=-\infty}^{\infty} c_k e^{il2\pi x_j/L} e^{-ik2\pi j/N} \tag{9.53}$$

$$= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{l=-\infty}^{\infty} c_k e^{il2\pi j/N} e^{-ik2\pi j/N} \tag{9.54}$$

$$= \sum_{l=-\infty}^{\infty} c_k \left(\frac{1}{N}\sum_{k=0}^{N-1} e^{i(l-k)2\pi j/N}\right) \tag{9.55}$$

$$\tag{9.56}$$

By the orthogonality relation, the sum is zero unless $l - j$ =multiples of integers, ie $l = k + mN$, where $m = 0, 1, 2, 3, ...$ Hence

$$\hat{u}^d_k = \sum_{l=-\infty}^{\infty} c_{k+mN} \tag{9.57}$$

This is something interesting: if we consider $u_1(x) = \cos(k2\pi x/L)$ and $u_2 = \cos((k+N)2\pi x/L$ and compute their Fourier series, then the first function will result in nonzero values only at $u^c_{\pm k}$ while the second function results in the exact same nonzeros. In other words, either function will yield the same right hand side. This phenomenon is known as "aliasing".

Now the question is: what is the useful information out of this infinite sum. To answer that question, we first assume that $k < \lfloor N/2 \rfloor$. Then out of all Fourier coefficients, k is the smallest index in the sum, whence c_k is the dominating term. We can see that from the re-written sum below

$$\hat{u}^d_k = c_k + \sum_{m=1}^{\infty} c_{k-mN} + \sum_{m=1}^{\infty} c_{k+mN} \tag{9.58}$$

On the other hand, assuming $\lfloor N/2 \rfloor \leq k \leq N$, we realize that c_{k-N} becomes the dominating coefficient. Hence, we write that

$$\hat{u}^d_k = c_{k-N} + \sum_{m=2}^{\infty} c_{k-mN} + \sum_{m=0}^{\infty} c_{k+mN} \tag{9.59}$$

Now what happens when $k = N/2$, for N even? Then there are two equally dominating terms in the sum, $c_{N/2}$ and $c_{N/2}$, which gives garbage. In summary

$$\hat{u}^d_k \approx \begin{cases} c_k, & 0 \leq k \leq \lfloor N/2 \rfloor \\ c_{k-N}, & \lfloor N/2 \rfloor < k \leq N \\ \text{garbage}, & k = N/2 \end{cases} \tag{9.60}$$

One may wonder if it is possible to just not pick N to be even and get away with thinking about $N/2$. In principle yes, but in practice, many methods, such as the fast Fourier transform, works the best for $N = 2^K$, for some integer K. Under this circumstance, N is even.

See codes for some demos of discrete Fourier transform.

9.5 Course Summary

We have certainly come a very long way. Throughout the summer, we have managed to cover many topics in computational mathematics, science and engineering. In particular, we have done

- Linear algebra and numerical linear algebra
- Spring-mass oscillations and ordinary differential equations
- Fourier series and Fourier transform

- Partial differential equations and analytic methods: separate of variables, Fourier transform
- Partial differential equations and numerical methods: finite difference, finite element
- Miscellaneous topics: DFT, heat equations, signal processing

Each topic has an infinite depth and we shall only illustrate a little bit of each

9.5.1 Linear algebra and numerical linear algebra

In a way, linear algebra is about solving the linear system,

$$Ax = b \tag{9.61}$$

for different kinds of matrices (eg. symmetric, positive definite, square, least square, etc). Going deeper, numerical linear algebra is definitely an interesting area to explore. A few interesting MIT courses for you to consider include

- 18.337 - Modern Numerical Computing
- 18.335J/6.337J: Introduction to Numerical Methods

An active area of research is parallel numerical linear algebra, that is, to perform analysis for parallel numerical linear algebra algorithms and/or design optimal numerical linear algebra well-suited for parallel programming approach

9.5.2 Spring-mass oscillations and ordinary differential equations

Spring-mass oscillation is a classic system that nonetheless finds its applications in numerous fields, from quantum mechanics and statistical mechanics to the designs of bridges and oil platform. Therefore, it is very important to gain a solid understanding of spring-mass systems.

The study of ordinary differential equations is also quite extensive, ranging from pure mathematics to applied physics and ecology. For example, the evolution of the equations on phase space can have some very enriching geometric properties. From a numerical standpoint, time-stepping is still an active area of research.

9.5.3 Fourier series and Fourier transform

This is a classic and beautiful area of mathematics that is more or less complete. Most of the research takes place in signal processing and compressed sensing. There are quite some theoretical development of harmonic analysis, which is a generalization of Fourier analysis, that is probably not of interest to engineers.

9.5.4 Partial differential equations and analytic methods

Analytic method is a fun topic. You would be surprised how far pencils and paper can get you in terms of significant insight into the behaviors of your systems. Separation of variables and Fourier transform are really just the tip of the iceberg. From a mathematical point of view, analysis can easily get quite abstract and pure, involving lots of rigorous arguments to prove existence and uniqueness.

9.5.5 Partial differential equations and numeric methods

This is a vast and active area of research that has been attracting billions of industry funding over the years. Aero-astro and mechanical engineering departments are both classic playgrounds of numerical partial differential equations. These days, the research tends to be focusing on equations involving stochastics.

A few other topics that you may wish to look into are

- Finite volume method
- discontinuous Galerkin method
- Spectral method (involving DFT)
- Spectral finite element method

9.5.6 Final Comments

If there is one missing piece from this class, that would be stochastic. Everything that we have dealt with so far is deterministic. There is no probability distributions or random variables anywhere. Things change for quite a bit when we add stochasticity to it.

Finally, everything that we have done so far is completely deductive: we start from the first principle and derive things from there. This is how mathematics should be done. Nonetheless, deductive approaches can be hard and slow, and thus we sometimes need a more top-down, inductive approach, for example, machine learning. This will be done by Prof. Gil Strang.

Last but not the least, I want to reiterate the purpose of this class. It is true that you may never have to compute the singular vectors of SVD by hand or know how to assemble the matrix of the finite element method beyond this course. But I am a firm believer of a solid foundation of knowledge. Even if you may be making business executive decisions for the rest of your careers, you may very likely take consolations in and appreciations of the subtle, rich, and beautiful mechanisms behind all the embellished front-ends.