Introduction to Finite Differences and FFT

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Overview

We will examine two numerical analysis techniques that can be used to find numerical solutions to differential equations. The first method is finite differences, and the second is the fast Fourier transform.

We obtain a system of algebraic equations through both of these techniques, and use linear algebra to solve the resulting matrix.

Using finite differences, we obtain a very large matrix because finite differences converge rather slowly. However, the good news is that it is highly structured and usually very sparse, lending itself to effective algorithms for the solution of sparse linear algebraic systems.

On the other hand, the fast Fourier transform is a method that converges very quickly, producing small matrices.

Finite Differences

The general idea behind finite differences is to replace derivatives with linear combinations of discrete function values.

We will first think about finite differences in terms of sequences indexed by all the integers.

$$z = \{z_k\}_{k=-\infty}^{k=\infty} = \dots, z_{-1}, z_0, z_1, \dots$$

Finite Difference Operators

Let us first define some elementary difference operators, which map the space R^Z of all such sequences into itself.

The Shift Operator

$(\mathcal{E}z)_k = z_{k+1}$

Example: $(\mathcal{E}\{z_1, z_2, z_3, ...\} = \{z_2, z_3, z_4, ...\}$
Essentially shifts a term forward to the next term.

The Forward Difference Operator

$(\Delta_+ z)_k = z_{k+1} - z_k$

That is, $(\Delta_+ z) = z_2 - z_1$
Difference between the next term and the current term

More Finite Difference Operators

The Backward Difference Operator

$(\Delta_{-} z)_k = z_k - z_{k-1}$

That is, $(\Delta_{-} z) = z_2 - z_1$
Difference between current term and the one before it

The Central Difference Operator

$(\Delta_0 z)_k = z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}$

More Finite Difference Operators

The Averaging Operator

$(\gamma_0 z)_k = \frac{1}{2}(z_{k-\frac{1}{2}} + z_{k+\frac{1}{2}})$

Note: The terms $z_{k+\frac{1}{2}}$ and $z_{k-\frac{1}{2}}$ do not make much sense for a sequence indexed by the integers, but when used appropriately, both the central difference operator and the averaging operator can be well defined.

The Differential Operator

Let us now assume that the sequence z is given by the sampling of a function z at equispaced points. In other words, $z_k = z(kh)$ for some constant $h > 0$.

Assuming that z is an entire function, meaning that z is a function that is complex differentiable at every point, we can define the differential operator as follows:

The Differential Operator

$(Dz)_k = z'(kh)$

General Definitions of Finite Difference Operators

Our next goal is to express the differential operator in terms of the other linear operators we have defined. In order to do this, we will formally define general functions of finite difference operators.

Since we assumed that $z_k = z(kh)$, finite difference operators depend on the parameter h.

Let

$$g(x) = \sum_{j=0}^{\infty} a_j x^j$$

be an arbitrary analytic function, expressed as its Taylor series.

General Definitions of Finite Difference Operators

Noting that

$$\mathcal{E} - \mathcal{I}, \gamma_0 - \mathcal{I}, \Delta_+, \Delta_-, \Delta_0, hD \to 0$$

when $h \to 0+$ and where $\mathcal{I}$ is the identity, we can formally expand g about $\mathcal{E} - \mathcal{I}, \gamma_0 - \mathcal{I}$, etc.

For example:

$$g(\Delta_+)z = (\sum_{j=0}^{\infty} a_j \Delta_+^j)z = \sum_{j=0}^{\infty} a_j(\Delta_+^j z)$$

The $\mathcal{E}^{\frac{1}{2}}$ Operator

$\mathcal{E}^{\frac{1}{2}}$ represents the square root of the shift operator.

One potential interpretation of its meaning is that is a "half-shift," meaning that $(\mathcal{E}^{\frac{1}{2}}z)_k = z_{k+\frac{1}{2}}$

We can also define this as $z((k+\frac{1}{2})h)$.

Definition of the $\mathcal{E}^{\frac{1}{2}}$ Operator

$(\mathcal{E}^{\frac{1}{2}}z)_k = z_{k+\frac{1}{2}}$

The $\mathcal{E}^{\frac{1}{2}}$ Operator

Another interpretation uses the power series expansion of $\sqrt{1+x}$ since the shift operator goes forward one term in the series z, and the $\mathcal{E}^{\frac{1}{2}}$ operator is the square root.

$$\sqrt{1+x} = 1 + \sum_{j=1}^{\infty} \left(\frac{(-1)^{j-1}}{2^{2j-1}} \right) \frac{(2j-2)!}{(j-1)!j!} x^j$$

implies that

Alternative Definition of the $\mathcal{E}^{\frac{1}{2}}$ Operator

$\mathcal{E}^{\frac{1}{2}} = \mathcal{I} - 2 \sum_{j=1}^{\infty} \frac{(2j-2)!}{(j-1)!j!} [-\frac{1}{4}(\mathcal{E} - \mathcal{I})]^j$

Expressing Operators as a Function of the Shift Operator

We will now express all finite difference operators in terms of the shift operator $\mathcal{E}$.

Since $(\mathcal{E}z)_k = z_{k+1}$ and $(\Delta_+ z)_k = z_{k+1} - z_k$,
$(\Delta_+ z)_k = z_{k+1} - z_k = (\mathcal{E}z)_k - z_k$

Therefore,

Forward Difference Operator

$\Delta_+ z = \mathcal{E} - \mathcal{I}$

Similarly,

Backward Difference Operator

$\Delta_- z = \mathcal{I} - \mathcal{E}^{-1}$

Expressing Operators as a Function of the Shift Operator

The definition of $\mathcal{E}^{\frac{1}{2}}$ as a half-shift implies that

Central Difference Operator

$\Delta_0 = \mathcal{E}^{\frac{1}{2}} - \mathcal{E}^{-\frac{1}{2}}$

Averaging Operator

$\gamma_0 = \frac{1}{2}(\mathcal{E}^{-\frac{1}{2}} + \mathcal{E}^{\frac{1}{2}})$

Expressing Operators as a Function of the Shift Operator

To express the differential operator in terms of the shift operator, we use the Taylor theorem.

For any analytic function z it is true that

$$
\begin{aligned}
\mathcal{E}z(x) = z(x+h) &= \sum_{j=0}^{\infty} \frac{1}{j!}[\frac{d^j z(x)}{dx^j}]h^j \\
&= [\sum_{j=0}^{\infty} \frac{1}{j!}(hD)^j]z(x) \\
&= e^{hD}z(x)
\end{aligned}
$$

Differential Operator

$D = \frac{1}{h}\ln\mathcal{E}$

Superposition of Finite Difference Operators

All of the previously mentioned operators are linear operators. Additionally, as they can be written in terms of $\mathcal{E}$, all six of them commute. Therefore when calculating the superposition of finite difference operators, the order is not important.

For example,

$$\begin{aligned}
\Delta_+\mathcal{E}^2 z_k &= \Delta_+(\mathcal{E}(\mathcal{E}z_k)) \\
&= \Delta_+(\mathcal{E}z_{k+1}) \\
&= \Delta_+ z_{k+2} \\
&= z_{k+3} - z_{k+2}
\end{aligned}$$

Expressing D in terms of Other Operators

We will first invert the above formulae to express $\mathcal{E}$ in terms of other operators.

Since $\Delta_+ = \mathcal{E} - \mathcal{I}$ and $\Delta_- = \mathcal{I} - \mathcal{E}^{-1}$

$$\mathcal{E} = \Delta_+ + \mathcal{I} = (\mathcal{I} - \Delta_-)^{-1}$$

Expressing D in terms of Other Operators

The expression involving Δ_0 is a quadratic equation for $\mathcal{E}^{\frac{1}{2}}$.

$$(\mathcal{E}^{\frac{1}{2}})^2 - \Delta_0 \mathcal{E}^{\frac{1}{2}} - \mathcal{I} = 0$$

After applying the quadratic formula, the solutions to this equation are

$$\mathcal{E}^{\frac{1}{2}} = \frac{1}{2}\Delta_0 \pm \sqrt{\frac{1}{4}\Delta_0^2 + \mathcal{I}}$$

Therefore,

$\mathcal{E} = (\frac{1}{2}\Delta_0 + \sqrt{\mathcal{I} + \frac{1}{4}\Delta_0^2})^2$

Expressing D in terms of Other Operators

Since $hD = \ln\mathcal{E}$, it follows that

The Differential Operator

$$
\begin{aligned}
D &= \frac{1}{h}\ln(\mathcal{I} + \Delta_+) \\
&= -\frac{1}{h}\ln(\mathcal{I} - \Delta_-) \\
&= \frac{2}{h}\ \ln(\frac{1}{2}\Delta_0 + \sqrt{\mathcal{I} + \frac{1}{4}\Delta_0^2})
\end{aligned}
$$

Approximation of the Differential Operator

As we are trying to approximate the differential operator D and its powers, we can expand the above formulae using the Taylor series for the natural log.

Using the formula for the differential operator in terms of the forward difference operator

$$
\begin{aligned}
D &= \frac{1}{h}\ln(\mathcal{I} + \Delta_+) \\
&= \frac{1}{h}[\Delta_+ - \frac{1}{2}\Delta_+^2 + \frac{1}{3}\Delta_+^3 + \mathcal{O}(\Delta_+^4)] \\
&= \frac{1}{h}(\Delta_+ - \frac{1}{2}\Delta_+^2 + \frac{1}{3}\Delta_+^3) + \mathcal{O}(h^3), \quad h \to 0
\end{aligned}
$$

Where we estimate $\Delta_+ = \mathcal{O}(h),\ h \to 0$

Approximation of the Differential Operator

If we apply this process s times, we get an expression for the sth derivative, where $s = 1, 2, 3, \ldots$

$$D^s = \frac{1}{h^s}[\Delta_+^s - \frac{1}{2}s\Delta_+^{s+1} + \frac{1}{24}s(3s+5)\Delta_+^{s+2}] + \mathcal{O}(h^3), \quad h \to 0$$

This means that the linear combination

$$\frac{1}{h^s}[\Delta_+^s - \frac{1}{2}s\Delta_+^{s+1} + \frac{1}{24}s(3s+5)\Delta_+^{s+2}]z_k$$

of the $s+3$ grid values $z_k, z_{k+1}, \ldots, z_{k+s+2}$ is an approximation for the sth derivative of $z(kh)$ up to O(h^3)

If we use only two terms instead of three, we would obtain order $\mathcal{O}(h^2)$, and expanding the series further would lead to higher order.

Approximation of the Differential Operator

We can also approximate the derivative using the backward difference operator, using grid points that lie all to the left. However, we would like to match the number of points on the left and right sides. Therefore we would now like to approximate the derivative using the central difference operator.

The problem with using the central difference operator is that $\Delta_0 z$ is not a proper grid sequence. As we noted before, terms like $z_{k+\frac{1}{2}}$ do not make much sense for a sequence indexed by the integers.

However, even powers of Δ_0 map the set of grid sequences to itself.

$$\Delta_0^2 z_n = z_{n-1} - 2z_n + z_{n+1}$$

Expressing the Differential Operator in terms of the Central Difference Operator

As we know, $D = \frac{2}{h}\ln(\frac{1}{2}\Delta_0 + \sqrt{\mathcal{I} + \frac{1}{4}\Delta_0^2})$

In order to obtain an expansion of this expression, let us consider the function $g(\mathcal{K}) = \ln(\mathcal{K} + \sqrt{1 + \mathcal{K}^2})$.

The Taylor expansion for this function is

$$g(\mathcal{K}) = 2\sum_{j=0}^{\infty} \frac{(-1)^j}{2j+1}\binom{2j}{j}(\frac{1}{2}\mathcal{K})^{2j+1}$$

$$\begin{aligned} D &= \frac{2}{h} g(\frac{1}{2}\Delta_0) \\ &= \frac{4}{h}\sum_{j=0}^{\infty} \frac{(-1)^j}{2j+1}\binom{2j}{j}(\frac{1}{4}\Delta_0)^{2j+1} \end{aligned}$$

Expressing the Differential Operator in terms of the Central Difference Operator

Unfortunately, the expression we obtained for D contains only odd powers of Δ_0. In order to obtain even powers of Δ_0, we can raise the expression to an even power.

Even Derivatives

$D^{2s} = \frac{1}{h^{2s}}[(\Delta_0^2)^s - \frac{s}{12}(\Delta_0^2)^{s+1} + \frac{s(11+5s)}{1440}(\Delta_0^2)^{s+2} - \frac{s(382+231s+35s^2)}{362880}(\Delta_0^2)^{s+3}] + \mathcal{O}(h^8), \quad h \to 0$

Therefore, the linear combination

$$\frac{1}{h^{2s}}[(\Delta_0^2)^s - \frac{s}{12}(\Delta_0^2)^{s+1} + \frac{s(11+5s)}{1440}(\Delta_0^2)^{s+2}]z_k$$

approximates $\frac{d^{2s}z(kh)}{dx^{2s}}$ to $\mathcal{O}(h^6)$.

Approximations of Odd Derivatives

The expansion described above only works for approximating even derivatives. In order to use the central difference operator to approximate odd derivatives, we will first express the averaging operator in terms of the central difference operator.

Since $(\gamma_0 z)_k = \frac{1}{2}(\mathcal{E}^{\frac{1}{2}} + \mathcal{E}^{-\frac{1}{2}})$ and $\Delta_0 = \mathcal{E}^{\frac{1}{2}} - \mathcal{E}^{-\frac{1}{2}}$
We can write

$$4\gamma_0^2 = \mathcal{E} + 2\mathcal{I} + \mathcal{E}^{-1}$$

$$\Delta_0^2 = \mathcal{E} - 2\mathcal{I} + \mathcal{E}^{-1}$$

And after some calculations, obtain

$$\gamma_0 = (\mathcal{I} + \frac{1}{4}\Delta_0^2)^{\frac{1}{2}}$$

Approximations of Odd Derivatives

Now we will write the identity $\mathcal{I}$ in terms of γ_0 and Δ_0.

$$\begin{aligned}\mathcal{I} &= \gamma_0(\gamma_0^{-1}) \\ &= \gamma_0(\mathcal{I} + \frac{1}{4}\Delta_0^2)^{-\frac{1}{2}}\end{aligned}$$

And now we will raise the original expansion of D using Δ_0 to an odd power, before multiplying by $\mathcal{I} = \gamma_0(\mathcal{I} + \frac{1}{4}\Delta_0^2)^{-\frac{1}{2}}$. This gives us

Odd Derivatives

$D^{2s+1} =$
$\frac{1}{h^{2s+1}}(\gamma_0\Delta_0)[(\Delta_0^2)^s - \frac{1}{12}(s+2)(\Delta_0^2)^{s+1} + \frac{1}{1440}(s+3)(5s+16)(\Delta_0^2)^{s+2}] + \mathcal{O}(h^5)$

where $h \to 0$

which is the recommended approximation of odd derivatives.

The Poisson Equation

The Poisson equation is a partial differential equation given by

The Poisson Equation

$\nabla^2 u = f, \quad (x, y) \in \Omega$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

$f = f(x, y)$ is a known continuous function and the domain $\Omega \subset \mathbb{R}$ is bounded, open and connected and has a piecewise-smooth boundary.

We will also assume the boundary condition

$$u(x, y) = \phi(x, y), \quad (x, y) \in \partial\Omega$$

In this case, $\partial\Omega$ denotes the boundary of the domain, and ϕ is a given function.

Using Grid Points

When using finite differences, we must always inscribe a grid onto the domain. We will now impose onto onto $\mathrm{cl}\Omega$ a square grid $\Omega_{\Delta x}$ parallel to the axes with squares of side length Δx.

Basically, we will choose $\Delta x > 0$, $(x_0, y_0) \in \Omega$ and let $\Omega_{\Delta x}$ be the set of all points $(x_0 + k\Delta x, y_0 + l\Delta x)$ inside the closure of Ω.

For convenience, we will notate the grid point $(x_0 + k\Delta x, y_0 + l\Delta x)$ as the (k, l)th grid point.

For every grid point (k, l) that lies within Ω, we will let $u_{k,l}$ represent the approximation to the solution $u(x_0 + k\Delta x, y_0 + l\Delta x)$ of the Poisson equation at that point.

We do not need to approximate the solution at any of the boundary points because their solutions are given by our boundary condition.

Types of Points

We will be using a formula that involves a linear combination of the five values $u_{k,l}$, $u_{k\pm1,l}$, $u_{k,l\pm1}$. This formula is only usable if the immediate horizontal and vertical neighbors (k, l) lie within Ω.

Let us define such a point $u(x_0 + k\Delta x, y_0 + l\Delta x)$ as an internal point.

A boundary point is a point that lies on $\partial\Omega$ and whose value is given by the boundary condition.

A near-boundary point is any other point inside clΩ. We cannot use finite differences to approximate the solutions to the PDE at these points.

Derivation of the Five-Point Formula

Suppose (k, l) corresponds to an internal point. We will use central differences in order to approximate its solution.

Let $v = v(x, y)$, $(x, y) \in \mathrm{cl}\Omega$, be an arbitrary sufficiently smooth function. Then at every internal grid point,

$$\frac{\partial^2 v}{\partial x^2} = \frac{1}{(\Delta x)^2}\Delta_{0,x}^2 v_{k,l} + \mathcal{O}((\Delta x)^2)$$

$$\frac{\partial^2 v}{\partial y^2} = \frac{1}{(\Delta x)^2}\Delta_{0,y}^2 v_{k,l} + \mathcal{O}((\Delta x)^2)$$

where $v_{k,l}$ is the value of v at the (k, l)th grid point.

This comes directly from the formula for finding even derivatives with the central difference operator we obtained earlier.

Derivation of the Five-Point Formula

We now see that

$$\frac{1}{(\Delta x)^2}(\Delta_{0,x}^2 + \Delta_{0,y}^2)$$

approximates ∇^2 to order $\mathcal{O}((\Delta x)^2)$.

This means that we can rewrite the Poisson Equation as

$$\frac{1}{(\Delta x)^2}(\Delta_{0,x}^2 + \Delta_{0,y}^2)u_{k,l} = f_{k,l}$$

at every internal grid point (k, l).

If we expand this by applying the operators, we obtain

The Five-Point Formula

$$u_{k-1,l} + u_{k+1,l} + u_{k,l-1} + u_{k,l+1} - 4u_{k,l} = (\Delta x)^2 f_{k,l}$$

Using the Five-Point Formula

So now instead of the original Poisson equation, we have a linear combination of the values of u at an internal grid point and the points immediately neighboring it.

Thus, the equation links five values of u in a linear fashion. However, unless any of the points lie on the boundary, their values are unknown.

We will now use the five-point formula to assign a linear equation to every internal grid point. This will give us a system of linear equations whose solution is our approximation $u_{k,l}$.

Fast Fourier Transform

As we said before, the fast Fourier transform is a method that converges quickly, requiring a smaller number of parameters. This results in a small matrix.

Before we begin looking at this method, we must first look at the approximation of functions.

We will use a Fourier series in order to approximate functions. The Fourier approximation is defined as follows:

Fourier Approximation

$f(x) \approx \varphi_N(x) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} f_n e^{i\pi nx}$

Where $f_n = \frac{1}{2}\int_{-1}^{1} f(\tau)e^{-i\pi n\tau}\,d\tau, \qquad n \in \mathbb{Z}$

The de la Valée Poussin Theorem

If the function f is Riemann integrable and $f_n = \mathcal{O}(n^{-1})$ for $|n| \gg 1$ then $\varphi_N(x) = f(x) + \mathcal{O}(n^{-1})$ as $n \to \infty$ for every point $x \in (-1, 1)$ where f is Lipschitz.

Lipschitz Functions

If a function is Lipschitz, there exists a real number such that, for every pair of points on the graph of this function, the absolute value of the slope of the line connecting them is not greater than this real number; the smallest such bound is called the Lipschitz constant of the function.

Note that if f is smoothly differentiable then, integrating by parts,

$$f_n = -\frac{(-1)^n}{2i\pi n}[f(1) - f(-1)] - \frac{1}{2i\pi n} f'_n = \mathcal{O}(n^{-1}), \quad |n| \gg 1$$

The Importance of Periodicity

Since such a function f is Lipschitz in (1, -1), φ_N converges to f there. However, unless f is periodic, it fails to converge to the correct values near the endpoints. Additionally, the convergence of $\mathcal{O}(n^{-1})$ is very slow.

However, when f is periodic, the Fourier approximation converges extremely quickly.

Suppose that f is an analytic function on $[-1, 1]$ that can be extended analytically to a closed complex domain Ω such that $[-1, 1] \subset \Omega$. Additionally, f is periodic with period 2.

Therefore $f^{(m)}(-1) = f^{(m)}(1)$ for all $m = 0, 1, \ldots$.

The Importance of Periodicity

We will again perform the integration, but this time we get

$$f_n = -\frac{1}{2\pi in} f'_n = (-\frac{1}{2\pi in})^2 f''_n = (-\frac{1}{2\pi in})^3 f'''_n = \dots$$

Therefore,

$$f_n = (-\frac{1}{2\pi in})^m f_n^{(m)}, \quad m = 0, 1, \dots$$

The Error Bound of the Fourier Approximation

How large is $|f^{(m)}|$? Let γ be the positively oriented boundary of Ω. The Cauchy theorem of complex analysis says that

$$f^{(m)}(x) = \frac{m!}{2\pi i} \int_{\gamma} \frac{f(z)dz}{(z-m)^{m+1}}, \qquad x \in [-1, 1]$$

After some steps, it follows that we can bound

$$f_n^{(m)} \leq cm!\alpha^m, \quad m = 0, 1, ..., \text{ for some } c > 0$$

. From this we can deduce that

$$|\varphi_n(x) - f(x)| \leq 3cm!(\frac{\alpha}{\pi N})^m$$

The Error Bound of the Fourier Approximation

According to the Stirling formula,

$$m! \approx \sqrt{2\pi} m^{m+1/2} e^{-m}$$

Therefore we have

$$m!(\frac{\alpha}{\pi N})^m \approx \sqrt{2\pi m}(\frac{\alpha m}{\pi e N})^m$$

which becomes very small for large N.

This means that the error $|\varphi_N - f|$ decays faster than $\mathcal{O}(N^{-p})$ for any $p = 1, 2, ...$

A rate of convergence of $\mathcal{O}(N^{-p})$ corresponds to order p, we say that the Fourier approximation of analytic periodic functions is of infinite order. This rapid convergence has a special name: we say that φ_N tends to f at spectral speed.

The Algebra of Fourier Expansions

Let us denote by $\mathcal{A}$ the set of all complex-valued functions f that are analytic in $[-1, 1]$ and can be extended analytically into the complex plane.

Suppose $f, g \in \mathcal{A}$ and $a \in \mathbb{C}$. Then f and g can be denoted with their convergent Fourier expansion as follows:

$$f(x) = \sum_{n=-\infty}^{\infty} f_n e^{i\pi nx}, \quad g(x) = \sum_{n=-\infty}^{\infty} g_n e^{i\pi nx}$$

The Algebra of Fourier Expansions

Addition of Fourier Expansions

$f(x) + g(x) = \sum_{n=-\infty}^{\infty} (f_n + g_n) e^{i\pi nx}$

Multiplication by a Constant

$af(x) = \sum_{n=-\infty}^{\infty} af_n e^{i\pi nx}$

Multiplication of Fourier Expansions

$f(x)g(x) = \sum_{n=-\infty}^{\infty} (\sum_{m=-\infty}^{\infty} f_{n-m} g_n) e^{i\pi nx}$

Derivatives of Fourier Expansions

$f'(x) = i\pi \sum_{n=-\infty}^{\infty} nf_n e^{i\pi nx}$

The Fast Fourier Transform

Let N be a positive integer and denote by Π_N the set of all complex sequences $x = \{x_j\}_{j=-\infty}^{\infty}$ which are periodic with period N, $j \in \mathbb{Z}$.

Π_N is a linear space of dimension N over the complex numbers $\mathbb{C}$.

Let $\omega_N = e^{2\pi i/N}$ be the Nth primitive root of unity.

The Primitive Root of Unity of Degree N

$\omega_N = e^{2\pi i/N}$

Discrete Fourier Transform

A discrete Fourier transform (DFT) is a linear mapping $\mathcal{F}_N$ defined for every $x \in \Pi_N$ by

Discrete Fourier Transform

$\mathbf{y} = \mathcal{F}_N \mathbf{x} \quad$ where $\quad y_j = \frac{1}{N} \sum_{\ell=0}^{N-1} \omega_N^{-j\ell} x_\ell, \quad j \in \mathbb{Z}$

The DFT defined above has some special properties. First, $\mathcal{F}_N$ maps Π_N into itself.

The mapping is also invertible and its inverse is given by

$$\mathbf{x} = \mathcal{F}_N^{-1} \mathbf{y} \quad \textit{where} \quad x_\ell = \frac{1}{N} \sum_{\ell=0}^{N-1} \omega_N^{j\ell} y_j, \quad \ell \in \mathbb{Z}$$

Additionally, $\mathcal{F}_N$ is an isomorphism of Π_N onto itself.

Evaluation of the DFT

At first glance, the evaluation of the DFT requires $\mathcal{O}(N^2)$ operations. This is because, owing to periodicity, it is obtained by multiplying a vector in $\mathbb{C}^N$ by a $N \times N$ complex matrix. However, the number of operations can be greatly reduced.

Let us assume that $N = 2^n$, where n is a nonnegative integer. We will also replace $\mathcal{F}_N$ by the mapping $\mathcal{F}_N^* = N\mathcal{F}_N$. If we can compute $\mathcal{F}_N^*\mathbf{x}$ cheaply then just $\mathcal{O}(N)$ operations will turn the result into $\mathcal{F}_N\mathbf{x}$.

Let us define, for every $\mathbf{x} \in \Pi_N$, "even" and "odd" sequences

$$\mathbf{x}^{[e]} := \{x_{2j}\}_{j=-\infty}^{\infty} \quad \textit{and} \quad \mathbf{x}^{[o]} := \{x_{2j+1}\}_{j=-\infty}^{\infty}$$

Evaluation of the DFT

Since $\mathbf{x}^{[e]}, \mathbf{x}^{[o]} \in \Pi_{N/2}$, we can make the mappings

$$\mathbf{y}^{[e]} = \mathcal{F}^*_{N/2}\mathbf{x}^{[e]} \quad \textit{and} \quad \mathbf{y}^{[o]} = \mathcal{F}^*_{N/2}\mathbf{x}^{[o]}$$

And find that

$$y_j = y_j^{[e]} + \omega_{2^n}^{-j\ell} y_j^{[o]} \qquad \text{for } j = 0, 1, ..., 2^n - 1$$

This means that if $\mathbf{y}^{[e]}$ and $\mathbf{y}^{[o]}$ are already known, we can synthesize them into $\mathbf{y}$ in $\mathcal{O}(N)$ operations.

Evaluation of the DFT

We can reduce the number of operations even further by using the identity $\omega_{2s}^{-s} = -1$ if $s \geq 1$.

$$y_j = y_j^{[e]} + \omega_{2^n}^{-j} y_j^{[o]}$$

$$y_{j+2^{n-1}} = y_{j+2^{n-1}}^{[e]} + \omega_{2^n}^{-j-2^{n-1}} y_{j+2^{n-1}}^{[o]} = y_j^{[e]} - \omega_{2^n}^{-j} y_j^{[o]}$$

This means we only need to calculate 2^{n-1} products $\omega_{2^n}^{-j} y_j^{[o]}$ and then subtract them from $y_j^{[e]}$ for $j = 0, 1, ..., 2^{n-1}$.

Similarly, we can find $\mathbf{y}^{[e]}$ by splitting it into "odd" and "even" sequences again. Then we can obtain $\mathbf{y}^{[e]}$ from two transforms of length $\frac{N}{4}$.

This process can be repeated until we reach transforms of unit length.

Implementation of FFT

The fast Fourier Transform begins with transforms of unit length and builds them up from there.

Assuming that $N = 2^n$ as we did previously, we begin with 2^n transforms of length 1 and synthesize them into 2^{n-1} transforms of length 2.

These are then combined into 2^{n-2} transforms of length 2^2, which are combined into 2^{n-3} transforms of length 2^3, and so on, until we reach a single transform of length 2^n, which is what we wanted in the first place.

This way, the cost of the FFT is $N\log_2 N$ operations, which is much faster than the original $\mathcal{O}(N^2)$ operations.

Spectral Methods

Spectral methods are useful because of the following phenomena:

The spectral convergence of Fourier expansions of analytic periodic functions,

The spectral convergence of a discrete Fourier transform approximation to Fourier coefficients of analytic periodic functions,

And the low-cost calculation of a DFT by the fast Fourier transform.

Second-Order Elliptic PDEs

Let us now use the fast Fourier transform to solve the Poisson equation. The special structure of a Poisson equation with periodic boundary conditions actually confers an advantage to spectral methods.

Specifically, consider the Poisson equation

$$\nabla^2 u = f, \quad -1 \leq x, y \leq 1$$

where the analytic function f obeys the periodic boundary conditions $f(-1, y) = f(1, y), -1 \leq y \leq 1$ and $f(x, -1) = f(x, 1), -1 \leq x \leq 1$.

We also have the periodic boundary conditions

$$u(-1, y) = u(1, y), \quad u_x(-1, y) = u_x(1, y), \quad -1 \leq y \leq 1$$

$$u(x, -1) = u(x, 1), \quad u_y(x, -1) = u_y(x, -1), \quad -1 \leq x \leq 1$$

Solution to Poisson Equation

We will also stipulate the normalization condition that

$$\int_{-1}^{1}\int_{-1}^{1} u(x,y)\mathrm{d}x\mathrm{d}y = 0$$

We have the two-dimensional Fourier expansion

$$f(x,y) = \sum_{k=-\infty}^{\infty}\sum_{\ell=-\infty}^{\infty} f_{k,\ell}e^{i\pi(kx+\ell y)}$$

And want to find the Fourier expansion of u

$$u(x,y) = \sum_{k=-\infty}^{\infty}\sum_{\ell=-\infty}^{\infty} u_{k,\ell}e^{i\pi(kx+\ell y)}$$

Solution to Poisson Equation

Because of the normalization condition, $u_{0,0} = 0$.

Therefore

$$\nabla^2 u(x,y) = -\pi^2 \sum_{k=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} (k^2 + \ell^2) u_{k,\ell} e^{i\pi(kx+\ell y)}$$

which implies that

$$u_{k,\ell} = -\frac{1}{(k^2+\ell^2)\pi^2} f_{k,\ell} \qquad k,\ell \in \mathbb{Z}, \quad (k,\ell) \neq (0,0)$$

Solution to Poisson Equation

We have obtained the Fourier coefficients of the solution explicitly, without needing to solve linear algebraic equations. This is because we have recreated numerically the technique of separation of variables.

The functions $\varphi_{k,\ell}(x, y) = e^{i\pi(kx+\ell y)}$ are eigenfunctions of the Laplace operator, $\nabla^2\varphi_{k,\ell} = -\pi^2(k^2 + \ell^2)_{k,\ell}$ and they obey periodic boundary conditions.