Finite Difference Method

Ayberk Nardan

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1 Calculus of Finite Difference

The motivation behind the calculus of finite differences is basically replacing derivatives with a linear combination of discrete function values.
We can consider the finite differences as a sequence of $\{z_k\}$, which can be complex or real. Then we introduce some operators on elements of this sequence called finite different operators.

Consider the element z_k as a function $z(kh)$ where the k is the step, and h is the length of equidistance discretization. Then, we can define the differentiation operator as

$$D(z_k) = z'(kh) \tag{1}$$

Our purpose is to write D in terms of the other operators. To achieve that purpose, we first need to define functions of operators as $g\mathcal{T}$. We will act such functions as if they are analytic functions, so they will have power series representation.

$$g(\mathcal{T}) = \sum_{i=0}^{\infty} a_i(T^i z)$$

Also, we need to define a half-shift operator to deal with fractional indexes.

$$\mathcal{E}^{\frac{1}{2}} z_k = z_{k+\frac{1}{2}} \tag{2}$$

Now consider $\mathcal{E}$ acts on $z(x)$

$$\mathcal{E} z(x) = z(x+h) \tag{3}$$

Operator	Operation
Shift Operator $:= \mathcal{E}$	$\mathcal{E}(Z_k) = z_{k+1}$
Forward Operator $:= \Delta_+$	$\Delta_+(z_k) = z_{k+1} - z_k$
Backward Operator $= \Delta_-$	$\Delta_-(z_k) = z_k - z_{k+1}$
Central Difference $:= \Delta_0$	$\Delta_0(z_k) = z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}$
Averaging Operator $:= \mathcal{T}_0$	$\mathcal{T}_0(z_k) = \frac{1}{2}(z_{k+\frac{1}{2}} + z_{k-\frac{1}{2}})$

Table 1: Table of the Operators

Then expansion of the $z(x)$ gives

$$\mathcal{E}z(x) = \sum \frac{1}{n!}\frac{d^n z}{dt^n}h^n \tag{4}$$

Replace the derivative with the operator D

$$\mathcal{E}z = \left(\sum \frac{1}{n!}(Dh)^n\right) z \tag{5}$$

Notice that there is the power series expansion of e^x in the RHS.

$$\mathcal{E}z = e^{(Dh)}z \tag{6}$$

$$ln(\mathcal{E}) = Dh \tag{7}$$

$$\Rightarrow D = \frac{1}{h}ln\mathcal{E} \tag{8}$$

Now one should notice that the basic operators can be written as linear combinations of the others. Three important representation of the $\mathcal{E}$ are

$$\mathcal{E} = \Delta_+ + I \tag{9}$$

$$\mathcal{E} = (\Delta_- + I)^{-1} \tag{10}$$

$$\tag{11}$$

The other one is the result of the following equation

$$\Delta_0 = \mathcal{E}^{\frac{1}{2}} - \mathcal{E}^{\frac{-1}{2}} \tag{12}$$

$$\Rightarrow \mathcal{E}^{\frac{1}{2}}\Delta_0 = (\mathcal{E}^{\frac{1}{2}})^2 - I \tag{13}$$

$$\mathcal{E}^{\frac{1}{2}} = \frac{\Delta_0}{2} + \sqrt{\frac{\Delta_0^2}{4} + I} \tag{14}$$

Then by taking the square of (14)

$$\mathcal{E} = \left(\frac{\Delta_0}{2} + \sqrt{\frac{\Delta_0^2}{4} + I}\right)^2 \tag{15}$$

Finally, we use these definitions of $\mathcal{E}$ in the equation (8) then Taylor expands the resulting function to obtain the differentiation operator. With definition (9), we get

$$D = \frac{1}{h}[\Delta_+ - \frac{1}{2}\Delta_+^2 + \frac{1}{3}\Delta_+^3] + \mathcal{O}(h^3) \tag{16}$$

and in general

$$D^s = \frac{1}{h^s}[\Delta_+^s - \frac{1}{2}s\Delta_+^{s+1} + \frac{s(3s+5)}{24}\Delta_+^{s+2}] + \mathcal{O}(h^3) \tag{17}$$

With this operator, we can differentiate a function up to an order $\mathcal{O}(h^3)$. Also, with the same procedure, one can find a formula with the Δ_- operator. The actual problem is to choose one. One should notice that the definition with the Δ_+ operator approximates the derivation using the elements $\{z_k, z_{k+1}, \cdots, z_{k+s+2}\}$. The Δ_- case on the other hand does the approximation using the points $\{z_k, z_{k-1}, \cdots, z_{k-s-2}\}$. The problem with such approximations is the fact that each operation uses only one side of the grids. A more proper approximation should have used both sides. This can be achieved by using the definition (15).
It gives the operator as

$$D = \frac{2}{h} ln \left(\frac{\Delta_0}{2} + \sqrt{I^2 + \left(\frac{\Delta_0}{4}\right)^2} \right) \tag{18}$$

To obtain a useful operation out of (18), lets us first consider the function

$$g(\epsilon) = ln(\epsilon + \sqrt{1+\epsilon^2}) \tag{19}$$

$$\Rightarrow g'(\epsilon) = \frac{1}{\sqrt{1+\epsilon^2}} = \sum (-1)^j \binom{2j}{j} \left(\frac{\epsilon}{2}\right)^{2j} \tag{20}$$

$g(0) = ln(1) = 0$. By the fundamental identity,

$$g(\epsilon) = g(0) + \int_0^\epsilon g'(t)dt \tag{21}$$

$$= 2 \sum \frac{(-1)^j}{2j+1} \binom{2j}{j} \left(\frac{\epsilon}{2}\right)^{2j+1} \tag{22}$$

$D = \frac{2}{h} g(\frac{\Delta_0}{2})$. Then the operation becomes

$$D = \frac{4}{h} \sum \frac{(-1)^j}{2j+1} \binom{2j}{j} \left(\frac{\Delta_0}{4}\right)^{2j+1} \tag{23}$$

The problem with this operator is all of the terms include odd powers of the central difference operator. Remember that Δ_0 cannot map $\mathbb{R}^z \to \mathbb{R}^z$. However, Δ_0^2 does.

$$\Delta_0^2 = \Delta_0(z_{k+\frac{1}{2}} - z_{k-1\frac{1}{2}}) \tag{24}$$

$$= z_{k+1} - 2z_k + z_{k-1} \tag{25}$$

Hence, we should consider the square of the operator (23). If we take the square and open the series up to some order, we get the following formula for the $2s$ derivative as

$$D^{2s} = \frac{1}{h^{2s}} [\Delta_0^{2s} - \frac{\Delta_0^{2s+2}}{12} + \frac{\Delta_0^{2s+4}}{45}] + \mathcal{O}(h^6) \tag{26}$$

We can obtain odd derivatives by defining an identity using the $\mathcal{T}_0$ operator.

$$\mathcal{T}_0 = \frac{1}{2}(\mathcal{E}^{\frac{1}{2}} + \mathcal{E}^{\frac{-1}{2}}) \tag{27}$$

$$\Rightarrow \mathcal{T}_0^2 = \frac{1}{4}(\mathcal{E} + \mathcal{E}^{-1} + 2I) \tag{28}$$

$\Delta_0^2 = \mathcal{E} + \mathcal{E}^{-1} - 2I$. Then some manipulation on (28) and Δ_0^2 gives following

$$\mathcal{T}_0 = \sqrt{I + \frac{\Delta_0^2}{4}} \Rightarrow I = \mathcal{T}_0 \left(I + \frac{\Delta_0^2}{4}\right)^{\frac{-1}{2}} \tag{29}$$

By the (20),

$$\left(I + \frac{\Delta_0^2}{4}\right)^{\frac{-1}{2}} = \sum(-1)^j \binom{2j}{j} \left(\frac{\Delta_0^2}{16}\right)^j \tag{30}$$

Consequently, we get the following identity

$$I = \mathcal{T}_0 \sum(-1)^j \binom{2j}{j} \left(\frac{\Delta_0^2}{16}\right)^j \tag{31}$$

Multiplying this identity with the differentiation operator (23) gives the following operator

$$D = \mathcal{T}_0 \Delta_0 \left(\sum(-1)^j \binom{2j}{j} \left(\frac{\Delta_0^2}{16}\right)^j\right) \left(\sum(-1)^i \binom{2i}{i} \left(\frac{\Delta_0^2}{16}\right)^i\right) \tag{32}$$

One can expand the series up to some order to get a useful differential operator. However, this is computationally wasteful and time consuming. For example, to get $\mathcal{O}^4$ order approximation, one will need seven grid points. A better way to get the D^{2s+1} operator is open the (23) to an odd order and then multiply it with the identity (29). This gives the following order six formula

$$D^{2s+1} = \frac{1}{h^{2s+1}}(\mathcal{T}_0\Delta_0)[\Delta_0^{2s} - \frac{(s+3)(5s+16)\Delta_0^{2s+2}}{12} + \frac{(s+3)(5s+16)\Delta_0^{2s+4}}{1440}] + \mathcal{O}(h^6) \tag{33}$$

2 The Five Point Formula

The Laplace equation is

$$\nabla^2 u(x,y) = f(x,y) \quad ,(x,y) \in \partial\Omega \tag{34}$$

where Ω is open, bounded, connected, and has a piecewise smooth boundary. To solve the equation, we also need a boundary condition just as we need for every other PDEs. Let's assume the Dirichlet Boundry condition.

$$u(x,y) = \phi(x,y), \quad (x,y) \in \partial\Omega \tag{35}$$

Now, we can impose a grid on the closure of Ω. Let the grid be parallel to the axis and let the space between two adjacent grid be $\Delta x > 0$ in both directions. Let $(x_0, y_0) \in \Omega$ be a point on the grid. Then we can define the set of all grid points as $\Omega_{\Delta x}$. The set of points is

$$I_{\Delta x} = \{(k,l) \in Z^2 : (x_0 + k\Delta x, y_0 + l\Delta x)\ incl(\Omega)\} \tag{36}$$

$$I^0 = \{(k,l) \in Z^2 : (x_0 + k\Delta x, y_0 + l\Delta x)\ in\Omega\} \tag{37}$$

Then we can denote the approximate solution at grid point $(k,l) \in I_{\Delta x}$ as

$$u_{k,l} = u(x_0 + k\Delta x, y_0 + l\Delta x) \tag{38}$$

We don't need to values of the solution on the boundary because it is given by the boundary condition. However, one should classify internal points as inner points and near boundary points, at least a neighbor point of which is a boundary point. At near boundary points, we no longer be able to use the finite differences method in general.
Now, we can focus on the Laplace operator.

$$\nabla^2 = \partial_x^2 + \partial_y^2 \tag{39}$$

We can approximate the partial derivatives using the D^{2s} definition (26).

$$D^{2s} = \frac{1}{h^{2s}}[\Delta_0^{2s} - \frac{\Delta_0^{2s+2}}{12} + \frac{\Delta_0^{2s+4}}{45}] + \mathcal{O}(h^6) \tag{40}$$

$$D^{2s} = \frac{1}{h^{2s}}\Delta_0^{2s} + \mathcal{O}(h^2) \tag{41}$$

$$D^{2s} = \frac{1}{h^2}\Delta_0^2 + \mathcal{O}(h^2) \tag{42}$$

Then the Poisson equation becomes the following form

$$\frac{1}{(\Delta x)^2}(\Delta_{0,x}^2 + \Delta_{0,y}^2)u_{k,l} = f_{k,l} \tag{43}$$

When we apply the operators, we reach the five point formula.

$$(\Delta x)^2 f_{k,l} = (U_{k+1,l} + U_{k-1,l} - U_{k,l} - U_{k,l}) + (U_{k,l+1} + U_{k,l-1} - U_{k,l} - U_{k,l}) \tag{44}$$

$$(\Delta x)^2 f_{k,l} = U_{k+1,l} + U_{k-1,l} + U_{k,l+1} + U_{k,l-1} - 4U_{k,l} \tag{45}$$

Notice that this formula turns our PDE into a set of linear equations. Let it be

$$Au = b \tag{46}$$

Then we have the important questions to trust our approximation

- Is the matrix A non-singular, so the solution u exists and is unique.
- Suppose such a u exists. Then do we have convergence?

To think about the questions lets Ω be square as

$$\Omega = \{(x, y) : 0 < x, y < 1\} \tag{47}$$

and boundary conditions

$$u(x, 0) = 0 \quad , u(x, 1) = \frac{1}{(1 + x)^2 + 1} \tag{48}$$

$$u(0, y) = \frac{y}{1 + y^2} \quad , u(1, y) = \frac{y}{4 + y^2} \tag{49}$$

Finally, let $(\Delta x)^2 f_{k,l} = F_{k,k}$. This setup gives the following linear equation. **Put the photo of the matrix.** By the equation (46), we have

$$\sum a_{k,l} u_{m,n} = f_{k,l} = u_{k+1,l} + u_{k-1,l} + u_{k,l+1} + u_{k,l-1} - 4u_{k,l} \tag{50}$$

Hence we have a relationship between the matrix elements and indices as

$$a_{k,l} = 1, \quad m = k + 1; n = l \tag{51}$$

$$a_{k,l} = 1, \quad m = k; n = l + 1 \tag{52}$$

$$a_{k,l} = -4, \quad k = k; n = l \tag{53}$$

Otherwise, it is zero. Notice that if $a_{k,l} = 0$ then $a_{l,k} = 0$ as well thanks to (51) and (52). Hence, we can conclude that the matrix A is symmetric
For the non-singularity, now let's consider the eigenvalues of the A. If we assume that the $v_{k,l}$ is an eigenvector of A as

$$v_{k,l} = sin\left(\frac{k\alpha\pi}{(m + 1)2}\right) sin\left(\frac{l\beta\pi}{(m + 1)2}\right) \tag{54}$$

The corresponding eigenvalue is

$$\lambda_{\alpha,\beta} = -4[sin^2\left(\frac{k\alpha\pi}{(m + 1)2}\right) + sin^2\left(\frac{l\beta\pi}{(m + 1)2}\right)] \tag{55}$$

which is always negative. Consequently, we reach the following theorem.

Theorem 2.1. *The matrix A is symmetric and negative definite. Hence, it is nonsingular.*

2.1 Error Analysis of the 5 Point Formula

Let $u(x, y)$ be the exact solution for the square grid Ω. Let $\tilde{u}_{k,l}$ be the exact solution at the point $(x_0 + k\Delta x, y_0 + l\Delta x)$ and $u_{k,l}$ be the corresponding approximation. Hence, we define the error as

$$e_{k,l} = |u_{k,l} - \tilde{u}_{k,l}| \tag{56}$$

Theorem 2.2. *For sufficiently smooth function f and boundary condition, there exist $c > 0$ that is independent of ΔX, such that*

$$\|e\| < c\Delta_x^2$$

The important point is that this theorem is valid only for grids that don't have near boundary points because the five point formula doesn't work for that points. The corrected formula for such cases is a six-point formula as

$$(\Delta_x)^2 f_{k,l} = \frac{\tau - 1}{\tau + 2} u_{k-2,l} + \frac{2(2-\tau)}{\tau + 1} u_{k-1,l} + \frac{6}{\tau(\tau+1)(\tau+2)} u_{k+\tau,l} + u_{k,l-1} + u_{k,l-1} - \frac{3+\tau}{\tau} u_{k,l} \tag{57}$$

where $\tau\Delta x$ is the distance between a near boundary point and a boundary point. This formula and the five-point formula gives the following theorem.

Theorem 2.3. *Let $Au{=}b$ be a linear system constructed with the five point formula for internal points and the six point formula for the near boundary points. Then the matrix A is non-singular. Hence, the method gives a unique solutions.*