Finite Difference Methods

Courant–Friedrichs–Lewy 1928

Lecture by Damian Sowinsk on 15 & 17 April 2014

1 Statement of the Problem

Our goal is to introduce how derivatives can be approximated by using difference quotients.

Suppose we have an interval $[a,b] \subset \mathbb{R}$. Let $a = x_0 < x_1 < \cdots < x_{N-1} < x_N = b$ be a partition. We call $\{x_1, \ldots, x_{N-1}\}$ the interior points, and $\{x_0, x_N\}$ the boundary. Given a function $f : [a,b] \to \mathbb{R}$, we want to approximate the derivative f' using our partition.

2 Difference Quotients

2.1 Definition

Based on the usual definition of the derivative, we can define an example of a difference quotient known as the forward difference.

(Definition) Forward Difference

$$D_+ f_i = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \tag{2.1}$$

There are a multitude of ways to define difference quotients. For example, we can also define the backward difference.

(Definition) Backward Difference

$$D_- f_i = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \tag{2.2}$$

2.2 Approximating the Derivative

We want to know how well these approximate the derivative of f in our problem statement. Consider,

$$D_+ f_i = \frac{f(x_i + \Delta x_i) - f(x_i)}{\Delta x_i} \tag{2.3}$$

$$\Delta x_i = x_{i+1} - x_i. \tag{2.4}$$

We can Taylor expand $D_+ f_i$ at a point x_i,

$$\begin{aligned} D_+ f_i &= \frac{1}{\Delta x_i}\left(f(x_i) + f'(x_i)\Delta x_i + \frac{1}{2} f''(x_i)\Delta x_i^2 + \mathcal{O}(\Delta x_i^3) - f(x_i)\right) \\ &= f'(x_i) + \frac{1}{2} f''(x_i)\Delta x_i + \mathcal{O}(\Delta x_i^2). \end{aligned} \tag{2.5}$$

We are left with an error, $\mathcal{O}(\Delta x_i)$, that is first order in Δx_i. The same holds if we repeat this with $D_- f_i$. Next, we want to modify this procedure to get an estimate that is better than $\mathcal{O}(\Delta x)$ in error.

2.3 Improving the Estimate

We can improve the estimate by using a difference quotient in the form of $Df_i = \sum_j a_j f_j$. The idea here is to use contraints in order to make the $f(x_i)$, $f'(x)\Delta x_i$ etc terms disappear in the Taylor expansion.

We illustrate this idea with an example that improves the previous error to $\mathcal{O}(\Delta x_i^2)$. Consider $af(x_i + \Delta x_i) + bf(x_i) + cf(x_i - \Delta x_{i-1})$. When we Taylor expand each of the $f(\cdot)$ term at the appropriate point, we get,

$$\begin{aligned} f(x_i + \Delta x_i) &= f(x_i) + f'(x_i)\Delta x_i + \frac{1}{2} f''(x_i)\Delta x_i^2 + \frac{1}{6} f'''(x_i)\Delta x_i^3 + \cdots \\ f(x_i) &= f(x_i) \\ f(x_i - \Delta x_{i-1}) &= f(x_i) - f'(x_i)\Delta x_{i-1} + \frac{1}{2} f''(x_i)\Delta x_{i-1}^2 - \frac{1}{6} f'''(x_i)\Delta x_{i-1}^3 + \cdots. \end{aligned} \tag{2.6}$$

This gives us a system of linear equations,

$$\begin{aligned} a + b + c &= 0, \\ a\Delta x_i + 0 - c\Delta x_{i-1} &= 0, \\ a\Delta x_i^2 + 0 + c\Delta x_{i-1}^2 &= 0. \end{aligned} \tag{2.7}$$

In matrix notation, we have,

$$\begin{pmatrix} 1 & 1 & 1 \\ \Delta x_i & 0 & -\Delta x_{i-1} \\ \Delta x_i^2 & 0 & \Delta x_{i-1}^2 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{2.8}$$

This gives us the difference quotient, $Df_i = \frac{\Delta x_{i-1}}{\Delta x} D_+ f_i + \frac{\Delta x_i}{\Delta x} D_- f_i$. In fact, we can approximate to whatever order we want by using this process.

If we let the length between each point of the partition be a constant h, i.e. $\Delta x_i = h$, then we have $\frac{f(x+h) - f(x-h)}{2h}$, which is the centered difference.

2.4 Approximating the nth Derivative

Now, suppose we want $D^n f_i$ with error $\mathcal{O}(\Delta x^2)$. With uniform spacing, i.e. $\Delta x_i = h$, we can keep applying our previous step.

$$
\begin{aligned}
Df_i &= \frac{1}{2h}\big(f(x+h) - f(x-h)\big), \\
D^2 f_i &= D\left[\frac{1}{2h}\big(f(x+h) - f(x-h)\big)\right], \\
&= \frac{1}{(2h)^2}\big(f(x+2h) - f(x) - f(x) + f(x-2h)\big), \\
&= \frac{1}{(h')^2}\big(f(x+h') - 2f(x) + f(x-h')\big),
\end{aligned} \tag{2.9}
$$

where $h' = 2h$. For an arbitrary even n, we have the formula,

$$
D^n f_i = \frac{1}{h^n}\sum_{m=0}^{n}\binom{n}{m}(-1)^m f_{i+(\frac{n}{2}-m)}. \tag{2.10}
$$

3 Accuracy of the Approximation

3.1 Example: Poisson's Equation

We consider Poisson's Equation: $\nabla^2 f = g$. In one dimension, this is just $\frac{d^2 f}{dx^2} = g$. We turn this into a finite difference equation by considering the centered difference quotient, $\frac{f_{i+1}-2f_i+f_{i-1}}{h^2} = g_i$. i.e. $D^2 f_i = \frac{1}{h^2}\big(f(x+h) - 2f(x) + f(x-h)\big)$.

Now, if our partition is $\{x_0, x_1, \ldots, x_{N-1}, x_N\}$, there are $N+1$ points including the boundary. Excluding the boundary points, this is a $N-1$ dimensional system of equations,

$$
\frac{1}{h^2}\begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -2 \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N-1} \end{pmatrix} = \begin{pmatrix} g_1 - \frac{\alpha}{h^2} \\ g_2 \\ \vdots \\ g_{N-1} - \frac{\beta}{h^2} \end{pmatrix}. \tag{3.1}
$$

Note that this is similar to what occurs in Hook's Law. We will write this system of equations as $AF = G$.

3.2 Local and Global Error

Let $\hat{F}$ be the actual solution to the differential equation, evaluated via f at the points in our partition. i.e. $\hat{F} = [f(x_1), \ldots, f(x_{N-1})]^T$. Then, there is a local truncation error τ such that,

$$
A\hat{F} = G + \tau. \tag{3.2}
$$

The global error, is $E = F - \hat{F}$. i.e. The difference between the solution to the finite difference equation and the actual solution to the differential equation. We can think of the local error as the “post" error, and the global error as the “pre" error.

3.3 Computing the Local Error

From above, we have $\tau = A\hat{F} - G$. So, the ith component of τ is,

$$\begin{aligned}
\tau_i &= \sum_j A_{ij} f(x_j) - g_i, \\
&= \frac{1}{h^2}\left(f(x_i) + f'(x_i)h + \frac{1}{2}f''(x_i)h^2 - 2f_i + f_i - f_i' h + \frac{1}{2}f_i'' h^2\right) - g_i, \\
&= \frac{1}{h^2}\left(\frac{1}{2}f''(x_i)h^2 + \frac{1}{2}f_i'' h^2\right) - g_i, \\
&= f''(x_i) + \frac{1}{12}h^2 f^4(x_i) + \mathcal{O}(h^4) - g(x_i)
\end{aligned} \tag{3.3}$$

Note that in the last step, the third order terms cancel. Using Poisson's Equation, we have $f'' = g$. So, $\tau_i = \frac{1}{12}h^2 f^4(x_i) + \mathcal{O}(h^4)$. Hence, the local truncation error is $\mathcal{O}(h^2)$.

3.4 Computing the Global Error

Next, we want to find the global error for Poisson's Equation using centered difference. From before, we know that the global error is $E = F - \hat{F}$. Note that $AE = AF - A\hat{F} = G - (G + \tau) \implies AE = -\tau$.

Look at the map $e(x_i) = E_i$, evaluated at a point x_i of our partition. Note that there is no error at the boundary points. i.e. $e(x_0) = e(x_N) = 0$. We have $e''(x) = -\frac{1}{12}h^2 f^4(x_i)$. Integrating twice, and again using $f'' = g$, we get $e(x_i) = -\frac{1}{12}g(x_i)h^2 + C_1 x + C_2$.

Using the boundary conditions, we can solve for the constants.

$$e(x_0) = 0 \implies -\frac{1}{12}g(x_0)h^2 + x_0 C_1 + C_2 = 0, \tag{3.4}$$

$$e(x_1) = 0 \implies -\frac{1}{12}g(x_N)h^2 + x_N C_1 + C_2 = 0. \tag{3.5}$$

This gives us,

$$C_1 = \frac{h^2}{12}\frac{g(x_0) - g(x_N)}{a - b}, \tag{3.6}$$

$$C_2 = \frac{h^2}{12}\frac{g(x_N) - g(x_0)}{a - b}. \tag{3.7}$$

In matrix notation, we have,

$$\begin{pmatrix} a & 1 \\ b & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \frac{h^2}{12}\begin{pmatrix} g(x_0) \\ g(x_N) \end{pmatrix}. \tag{3.8}$$

Therefore, the global error $||e(x)||_2 \to 0$ as $h \to 0$.

4 Neccessary Conditions for Convergence

We want to show conditions under which the global error $||E|| \to 0$ as $h \to 0$ generally.

Suppose one has a finite difference method for a linear boundary value problem that gives a sequence $A_h F_h = G$ where, $h = \frac{1}{N-1}$. So, h is smaller when the dimension N is larger.

(Definition) Stable

The method is stable if $(A^h)^{-1}$ exists for all h sufficiently small, and there exists a $c \in \mathbb{R}$ independent of h such that,

$$||(A^h)^{-1}|| \leq C \text{ for all } h \leq h_0, \tag{4.1}$$

for some h_0. i.e. For h “small" enough. Intuitively, stability is how close the finite difference solution is to the actual PDE solution.

(Definition) Consistent

The method is consistent with the differential equations and boundary conditions if,

$$||\tau^h|| \to 0 \text{ as } h \to 0. \tag{4.2}$$

Intuitively, consistency is how closely the finite difference method is satisfied by the actual solutions to the differential equations.

(Theorem) The Fundamental Theorem of Finite Differences

Consistency and stability implies convergence.

(Proof) $A^h E^h = -\tau^h \implies E^h = (A^h)^{-1}\tau^h \implies ||E^h|| = ||(A^h)^{-1}\tau^h|| \leq ||(A^h)^{-1}||||\tau^h|| \leq C||\tau^h|| \to 0.$

4.1 Convergence under Different Norms

We know that norms are equivalent in finite dimensional vector spaces. Therefore, this works for any norms. However, the scalar factor will be different.

Note that if the local truncation error $||\tau^h||$ is $\mathcal{O}(h^p)$, then the global error $||E^h||$ is $\mathcal{O}(h^p)$ regardless of norm, since the norms differ only by a constant.

5 Convergence for Poisson's Equation

Suppose we have a system of equations for the one dimensional Poisson's Equation, $FU = G$. Note that the notation has changed from the $AF = G$ used previously. We want to prove its convergence explicitly.

Since F is a symmetric matrix, the operator norm (or 2-norm) is $||F||_2 = \max_p |\lambda_p|$, where the maximum is taken over all the eigenvalues of F. This is also known as the spectral radius of F. Then, we have $||F^{-1}||_2 = \max_p |\lambda_p^{-1}| = (\min_p |\lambda_p|)^{-1}$.

(Claim) $F^h(u_p) = \lambda_p^h u_p^h$, where $u_p = \sum_j \hat{e}_j \sin(p\pi jh)$, and $\lambda_p = \frac{2}{h^2}(\cos(p\pi h) - 1)$ are respectively the eigenvectors and eigenvalues of F.

(Proof)

$$\begin{aligned}
F(u_p) &= \frac{1}{h^2}\sum_i \hat{e}_i \left(u_{i+1}^p - 2u_i^p + u_{i-1}^p\right), \\
&= \frac{1}{h^2}\sum_{i,j} \hat{e}_i \left(\sin(p\pi(i+1)h) - 2\sin(p\pi ih) + \sin(p\pi(i-1)h)\right) \\
&= \frac{1}{h^2}\sum_i \hat{e}_i \left(\sin\theta i\cos\theta + \sin\theta\cos\theta - 2\sin\theta i + \sin\theta i\cos\theta - \sin\theta\cos\theta\right), \\
&= \frac{1}{h^2}\sum_i \hat{e}_i \sin\theta i(2\cos\theta - 2), \\
&= \frac{2}{h^2}(\cos(\pi ph) - 1)\sum_i \hat{e}_i \sin(p\pi ih), \\
&= \lambda_p u_p.
\end{aligned} \tag{5.1}$$

where we let $\theta = \pi ph$ to simplify the manipulations, and we used the angle sum formula from trigonometry. Therefore, we have,

$$\begin{aligned}
||F^{-1}||_2 &= \left(\frac{2}{h^2}(\cos\pi ph - 1)\right)^{-1}, \\
&= \left[\frac{2}{h^2}(1 - \{1 - \frac{1}{2}\pi^2h^2 + \mathcal{O}(h^4)\})\right]^{-1}, \\
&= (\pi^2 + \mathcal{O}(h^2))^{-1},
\end{aligned} \tag{5.2}$$

which goes to $\frac{1}{\pi^2}$ as $h \to 0$. Finally,

$$||E^h||_2 \le ||(F^h)^{-1}|| |\tau^h|_2 \le \frac{1}{\pi^2}\frac{1}{12}||g''||_2 h^2 \tag{5.3}$$

where we used our result for τ from (3.1), and that $f'' = g$. So, as long as the source function g is C^2, the one dimensional Poisson's Equation is convergent. i.e. (5.3) goes to 0, as h goes to 0.

6 Extending to the Two Dimensional Case

6.1 Definitions and Setup

Consider the lattice $L = \{(nh, mh) \mid n, m \in \mathbb{Z}, h \in \mathbb{R}^+\}$ with spacing size h. Let Ω be the region in $\mathbb{R}^2$ such that $\partial\Omega$ is closed, continuous and has no double point.

Define the mesh $\Omega_h = \Omega \cap L = \Omega'_h \cup \partial\Omega_h$, where Ω'_h is the interior and $\partial\Omega_h$ is the boundary. The interior are all points on the lattice such that all their neighbors are also in Ω_h. The boundary are points such that some neighbors are not in Ω_h.

Next, we define a bilinear form using forward difference,

$$
\begin{aligned}
B(u,v) = & aD_x(u)D_x(v) + bD_x(u)D_y(v) + cD_y(u)D_x(v) + dD_y(u)D_y(v) \\
& + \alpha D_y(u)v + \beta D_y(u)v + \gamma uD_x(v) + \delta uD_y(v) + guv.
\end{aligned} \tag{6.1}
$$

This is analogous to a Lagrangian for the continuous case. Now, we want to sum this over all the mesh grid points. We construct a discrete "action",

$$
S^h = h^2 \sum_{\Omega_h} B(u,v) = \begin{cases} -h^2 \sum_{\Omega'_h} vL(u) + h \sum_{\partial\Omega_h} vR(u) \\ -h^2 \sum_{\Omega'_h} uM(v) + h \sum_{\partial\Omega_h} uS(v). \end{cases} \tag{6.2}
$$

So, the sum decompose into a sum over interior points and a sum over boundary points. Now, we want to know what $L(u)$ looks like. Note that $h\sum_{\Omega_h} uD_x(v) = \sum_{\partial\Omega_h} vR(u) - h\sum_{\Omega'_h} v\hat{D}_x(u)$. So, we have $L(u) = \hat{D}_x(aD_x(u)) + \hat{D}_y(bD_x(u)) + \cdots - \hat{D}_x(\alpha D_x(u)) \cdots + \hat{D}_x(\gamma(u)) - gu$.

6.2 Symmetric Case

For simplicity, we restrict our attention to when B is symmetric. i.e. $B(u,v) = B(v,u)$. Then, $b = c$, $\alpha = \gamma$, $\beta = \delta$ in (6.1). Also, $L = M$ and $R = S$ in (6.2). Then, we have,

$$
\begin{aligned}
B(u,u) = & [a(D_x(u))^2 + 2b\hat{D}_x(u)D_y(u) + c(D_y(u))^2] \\
& + 2\alpha uD_x(u) + 2\beta uD_y(u) + gu^2.
\end{aligned} \tag{6.3}
$$

Let $p(u,u) = a(D_x(u))^2 + 2b\hat{D}_x(u)D_y(u) + c(D_y(u))^2$. We call this the characteristic form. If $p(u,u)$ is semi-definite in finite differences, then we say B is elliptic. If $p(u,u)$ is not semi-definite, we say B is hyperbolic. Treating this like a minimization problem, we have,

$$
S[\phi] = h^2 \sum_{\Omega_h} B(\phi,\phi), \tag{6.4}
$$

$$
u = \text{argmin}_\phi S[\phi] \implies L(u) = 0. \tag{6.5}
$$

If we perturb $\phi \to \phi + \delta\phi$, then $S[\phi] \to S[\phi + \delta\phi]$, we get,

$$
\begin{aligned}
S[\phi + \delta\phi] &= h^2 \sum_{\Omega_h} B(\phi + \delta\phi, \phi + \delta\phi) \\
&= S[\phi] + 2h^2 \sum_{\Omega_h} B(\phi, \delta\phi) + \mathcal{O}(\delta\phi^2) \\
&= S[\phi] + 2h^2 \sum_{\Omega'_h} \delta\phi L(\phi) + \sum_{\partial\Omega_h} \delta\phi R(\phi)
\end{aligned} \tag{6.6}
$$

Now, $\sum_{\partial\Omega_h} \delta\phi R(\phi) = 0$ since the variation on the boundary is 0. So, $L(\phi)$ must be identically 0.

6.3 Conditions for Convergence

For convergence, given any $\Omega^* \subset \Omega$, we need u_n and all of its finite differences to be bounded and equicontinuous.

Equicontinuity means that for each function w_h, there is a $\delta(\epsilon)$ such that $|P - P_1| < \delta(\epsilon) \implies |w_h(P) - w_h(P_1)| < \epsilon$, for all h.

The proof of convergence roughly consists of these three steps,

1. $h \to 0$, $h^2 \sum u^2$ and $h^2 \sum (D_x(u))^2 + (D_y(u))^2$ have to be bounded.
2. Recursive reasoning show that all the difference quotients are bounded.
3. Boundedness of all DQ $\implies$ equicontinuity.

We give a proof of the first step. The solution satisfies the Laplacian $\Delta u = 0$ and so it must be on the boundary. Now, $h^2 \sum (D_x(u))^2 + (D_y(u))^2 \le h^2 \sum (D_x(g))^2 + (D_y(g))^2$, where g is a function that satisfies the partial differential equation and boundary condition. However, $\int dA (\frac{\partial g}{\partial x})^2 + (\frac{\partial g}{\partial y})^2 = C$.

Therefore, $h^2 \sum (D_x(u))^2 + (D_y(u))^2$ is bounded by C.

7 Wave Equation Example

Consider the equation,

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}. \tag{7.1}$$

We can intrepret this as “acceleration is propotional to curvature". Note that this is hyperbolic because manipulating it into $\frac{\partial^2 y}{\partial t^2} - c^2 \frac{\partial^2 y}{\partial x^2} = 0$ results in a negative sign. We turn this into a finite difference model,

$$\frac{y_i^{t+1} - 2y_i^t + y_i^{t+1}}{\Delta t^2} = c^2 \frac{y_{i-1}^t - 2y_i^t + y_{i-1}^t}{\Delta x^2}. \tag{7.2}$$

This can be manipulated into,

$$\begin{aligned} y_i^{t+1} &= 2y_i^t - y_i^{t-1} + c^2 \frac{\Delta t^2}{\Delta x^2}(y_{i+1}^t - 2y_i^t + y_{i-1}^t), \\ &= 2(1 - c^2 \frac{\Delta t^2}{\Delta x^2}) y_i^t + c^2 \frac{\Delta t^2}{\Delta x^2}(y_{i+1}^t + y_{i-1}^t) - y_i^{t-1}. \end{aligned} \tag{7.3}$$

We let $\Delta x = \Delta t$. i.e. We make the grid spacing for both time and space equal. In rough matrix notation, we have,

$$\begin{pmatrix} \\ Y \\ \\ \end{pmatrix}^{t+1} = \begin{pmatrix} 2(\frac{1}{c^2}-1) & 1 & 0 & \cdots \\ 1 & 2(\frac{1}{c^2}-1) & 1 & \cdots \\ 0 & 1 & 2(\frac{1}{c^2}-1) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \\ Y \\ \\ \end{pmatrix}^{t} - \begin{pmatrix} \\ Y \\ \\ \end{pmatrix}^{t-1}. \tag{7.4}$$

This is similar to (3.1), which we noticed was analogous to a system of springs. From what we know about springs and Hook's Law, we need $(\frac{1}{c^2}-1) < 0 \implies c > 1$. We can interpret c as the speed of information progation. If c is not large enough, the system is unstable. However, if $c > 1$, we get the wave behavior that we were expecting*.

*This was demonstrated using the computer during the lecture.