FINITE DIFFERENCE METHODS

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The best known methods, finite difference, consists of replacing each derivative by a difference quotient in the classic formulation. It is simple to code and economic to compute. In a sense, a finite difference formulation offers a more direct approach to the numerical solution of partial differential equations than does a method based on other formulations. The drawback of the finite difference methods is accuracy and flexibility. Standard finite difference methods requires more regularity of the solution (e.g. $u \in \mathcal{C}^2(\Omega)$) and the triangulation (e.g. uniform grids). Difficulties also arises in imposing boundary conditions.

1. Finite difference formula

In this section, for simplicity, we discuss Poisson equation posed on the unit square $\Omega = (0,1) \times (0,1)$. Variable coefficients and more complex domains will be discussed in finite element methods. Furthermore we assume u is smooth enough to enable us use Taylor expansion freely.

Given two integer $m, n \geq 2$, we construct a rectangular grids $\mathcal{T}_h$ by the tensor product of two grids of $(0,1)$: $\{x_i = (i-1)h_x, i = 1, \cdots m, h_x = 1/(m-1)\}$ and $\{y_j = (j-1)h_y, j = 1, \cdots n, h_y = 1/(n-1)\}$. Let $h = \max\{h_x, h_y\}$ denote the size of $\mathcal{T}_h$. We denote $\Omega_h = \{(x_i, y_j) \in \Omega\}$ and boundary $\Gamma_h = \{(x_i, y_j) \in \partial\Omega\}$.

We consider the discrete function space given by $\mathbb{V}_h = \{u_h(x_i, y_j), 1 \leq i \leq m, 1 \leq j \leq n\}$ which is isomorphism to $\mathbb{R}^N$ with $N = m \times n$. It is more convenient to use sub-index (i,j) for the discrete function: $u_{i,j} := u_h(x_i, y_j)$. For a continuous function $u \in \mathcal{C}(\Omega)$, the interpolation operator $I_h : \mathcal{C}(\Omega) \to \mathbb{V}_h$ maps u to a discrete function and will be denoted by u_I. By the definition $(u_I)_{i,j} = u(x_i, y_j)$. Note that the value of a discrete function is only defined at grid points. Values inside each cell can be obtained by interpolation of values at grid points.

Similar definitions can be applied to one dimensional case. Choose a mesh size h and $u \in \mathbb{V}_h(0,1)$. Popular difference formulas at an interior node x_j for a discrete function $u \in \mathbb{V}_h$ include:

- The backward difference: $(D^- u)_j = \dfrac{u_j - u_{j-1}}{h}$;
- The forward difference: $(D^+ u)_j = \dfrac{u_{j+1} - u_j}{h}$;
- The centered difference: $(D^\pm u)_j = \dfrac{u_{j+1} - u_{j-1}}{2h}$;
- The centered second difference: $(D^2 u)_j = \dfrac{u_{j+1} - 2u_j + u_{j-1}}{h^2}$.

It is easy to prove by Talyor expansion that

$$
\begin{aligned}
(D^- u)_j - u'(x_j) &= \mathcal{O}(h), & (D^+ u)_j - u'(x_j) &= \mathcal{O}(h), \\
(D^\pm u)_j - u'(x_j) &= \mathcal{O}(h^2), & (D^2 u)_j - u''(x_j) &= \mathcal{O}(h^2).
\end{aligned}
$$

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We shall use these difference formulation, especially the centered second difference to approximate the Laplace operator at an interior node (x_i, y_j):

$$\begin{aligned}(\Delta_h u)_{i,j} &= (D^2_{xx}u)_{i,j} + (D^2_{yy}u)_{i,j}\\ &= \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,i}}{h_x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h_y^2}.\end{aligned}$$

It is called five point stencil since only five points are involved. When $h_x = h_y$, it is simplified to

$$-(\Delta_h u)_{i,j} = \frac{4u_{i,j} - u_{i+1,j} - u_{i-1,i} - u_{i,j+1} - u_{i,j-1}}{h^2} \tag{1}$$

and can be denoted by the following stencil symbol

$$\begin{pmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{pmatrix}.$$

For the right hand side, we simply take node values i.e. $f_{i,j} = (f_I)_{i,j} = f(x_i, y_j)$.

The finite difference methods for solving Poisson equation is simply

$$-(\Delta_h u)_{i,j} = f_{i,j}, \quad 1 \le i \le m, 1 \le j \le n, \tag{2}$$

with appropriate processing of boundary conditions. Here in (2), we also use (1) for boundary points but drop terms involving grid points outside of the domain.

Let us give an ordering of $N = m \times n$ grids and use a single index $k = 1$ to N for $u_k = u_{i(k),j(k)}$. For example, the index map $k \to (i(k), j(k))$ can be easily written out for the lexicographical ordering. With any choosing ordering, (2) can be written as a linear algebraic equation:

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}, \tag{3}$$

where $\boldsymbol{A} \in \mathbb{R}^{N\times N}$, $\boldsymbol{u} \in \mathbb{R}^N$ and $\boldsymbol{f} \in \mathbb{R}^N$.

Remark 1.1. There exist different orderings for the grid points. Although they give equivalent matrixes up to permutations, different ordering does matter when solving linear algebraic equations.

2. Boundary conditions

We shall discuss how to deal with boundary conditions in finite difference methods. The Dirichlet boundary condition is relatively easy and the Neumann boundary condition requires the ghost points.

Dirichlet boundary condition. For the Poisson equation with Dirichlet boundary condition

$$-\Delta u = f \text{ in } \Omega, \quad u = g \text{ on } \Gamma = \partial\Omega, \tag{4}$$

the value on the boundary is given by the boundary conditions. Namely $u_{i,j} = g(x_i, y_j)$ for $(x_i, y_j) \in \partial\Omega$ and thus not unknowns in the equation. There are several ways to impose the Dirichlet boundary condition.

One approach is to let $a_{ii} = 1, a_{ij} = 0, j \neq i$ and $f_i = g(x_i)$ for nodes $x_i \in \Gamma$. Note that this will destroy the symmetry of the corresponding matrix. Another approach is to modify the right hand side at interior nodes and solve only equations at interior nodes. Let us consider a simple example with 9 nodes. The only unknowns is u_5 with the lexicographical ordering. By the formula of discrete Laplace operator at that node, we obtain the adjusted equation

$$\frac{4}{h^2}u_5 = f_5 + \frac{1}{h^2}(u_2 + u_4 + u_6 + u_8).$$

We use the following Matlab code to illustrate the implementation of Dirichlet boundary condition. Let `bdNode` be a logic array representing boundary nodes: `bdNode(k)=1` if $(x_k, y_k) \in \partial\Omega$ and `bdNode(k)=0` otherwise.

```
freeNode = ~bdNode;
u = zeros(N,1);
u(bdNode) = g(node(bdNode,:));
f = f-A*u;
u(freeNode) = A(freeNode,freeNode)\f(freeNode);
```

The matrix `A(freeNode,freeNode)` is symmetric and positive definite (SPD) (see Exercise 1) and thus ensure the existence of the solution.

Neumann boundary condition. For the Poisson equation with Neumann boundary condition

$$-\Delta u = f \ \text{ in } \Omega, \quad \frac{\partial u}{\partial n} = g \text{ on } \Gamma,$$

there is a compatible condition for f and g:

$$\int_\Omega f\,dx = -\int_\Omega \Delta u\,dx = \int_{\partial\Omega} \frac{\partial u}{\partial n}\,dS = \int_{\partial\Omega} g\,dS. \tag{5}$$

A natural approximation to the normal derivative is a one sided difference, for example:

$$\frac{\partial u}{\partial n}(x_1, y_j) = \frac{u_{1,j} - u_{2,j}}{h} + O(h).$$

But this is only a first order approximation. To treat Neumann boundary condition more accurately, we introduce the ghost points outside of the domain and next to the boundary.

We extend the lattice by allowing the index $0 \le i, j \le n+1$. Then we can use center difference scheme:

$$\frac{\partial u}{\partial n}(x_1, y_j) = \frac{u_{0,j} - u_{2,j}}{2h} + O(h^2).$$

The value $u_{0,j}$ is not well defined. We need to eliminate it from the equation. This is possible since on the boundary point (x_1, y_j), we have two equations:

$$4u_{1,j} - u_{2,j} - u_{0,j} - u_{1,j+1} - u_{1,j-1} = h^2 f_{1,j} \tag{6}$$

$$u_{0,j} - u_{2,j} = 2h\, g_{1,j}. \tag{7}$$

From (7), we get $u_{0,j} = 2h\, g_{1,j} + u_{2,j}$. Substituting it into (6) and scaling by a factor $1/2$, we get an equation at point (x_1, y_j):

$$2u_{1,j} - u_{2,j} - 0.5\, u_{1,j+1} - 0.5\, u_{j-1} = 0.5\, h^2 f_{1,j} + h\, g_{1,j}.$$

The scaling is to preserve the symmetry of the matrix. We can deal with other boundary points by the same technique except the four corner points. At corner points, even the norm vector is not well defined. We will use average of two directional derivatives to get an approximation. Taking $(0, 0)$ as an example, we have

$$4u_{1,1} - u_{2,1} - u_{0,1} - u_{1,1} - u_{1,0} = h^2 f_{1,1}, \tag{8}$$

$$u_{0,1} - u_{2,1} = 2h\, g_{1,1}, \tag{9}$$

$$u_{1,0} - u_{1,2} = 2h\, g_{1,1}. \tag{10}$$

So we can solve $u_{0,1}$ and $u_{1,0}$ from (9) and (10), and substitute them into (8). Again to maintain the symmetric of the matrix, we multiply (8) by $1/4$. This gives an equation for the corner point (x_1, y_1)

$$u_{1,1} - 0.5\, u_{2,1} - 0.5\, u_{1,1} = 0.25\, h^2 f_{1,1} + h\, g_{1,1}.$$

Similar technique will be used to deal with other corner points. We then end with a linear algebraic equation

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}.$$

It can be shown that the corresponding matrix $\boldsymbol{A}$ is still symmetric but only semi-definite (see Exercise 2). The kernel of $\boldsymbol{A}$ consists of constant vectors i.e. $\boldsymbol{A}\boldsymbol{u} = 0$ if and only if $\boldsymbol{u} = c$. This requires a discrete version of the compatible condition (5):

$$\sum_{i=1}^{N} f_i = 0 \tag{11}$$

and can be satisfied by the modification `f = f - mean(f)`.

3. Error estimate

In order to analyze the error, we need to put the problem into a norm space. A "natural" norm for the finite linear space $\mathbb{V}_h$ is the maximum norm: for $v \in \mathbb{V}_h$,

$$\|v\|_{\infty,\Omega_h} = \max_{\substack{1 \le i \le n+1,\\ 1 \le j \le m+1}} \{|v_{i,j}|\}.$$

The subscript h indicates this norm depends on the triangulation since for different h, we have different numbers of $v_{i,j}$. Note that this is the l^∞ norm for $\mathbb{R}^N$.

We shall prove $\Delta_h^{-1} : (\mathbb{V}_h, \|\cdot\|_{\infty,\Omega_h}) \to (\mathbb{V}_h, \|\cdot\|_{\infty,\Omega_h})$ is stable uniform to h. The proof will use the discrete maximal principal and barrier functions.

Theorem 3.1 (Discrete Maximum Principle). *Let $v \in \mathbb{V}_h$ satisfy*

$$\Delta_h v \ge 0.$$

Then

$$\max_{\Omega_h} v \le \max_{\Gamma_h} v,$$

and the equality holds if and only if v is constant.

Proof. Suppose $\max_{\Omega_h} v > \max_{\Gamma_h} v$. Then we can take an interior node x_0 where the maximum is achieved. Let x_1, x_2, x_3, and x_4 be the four neighbors used in the stencil. Then

$$4v(x_0) = \sum_{i=1}^{4} v(x_i) - h^2 \Delta_h v(x_0) \le \sum_{i=1}^{4} v(x_i) \le 4v(x_0).$$

Thus equality holds throughout and v achieves its maximum at all the nearest neighbors of x_0 as well. Applying the same argument to the neighbors in the interior, and then to their neighbors, etc, we conclude that v is constant which contradicts to the assumption

$\max_{\Omega_h} v > \max_{\Gamma_h} v$. The second statement can be proved easily by a similar argument. $\square$

Theorem 3.2. *Let u_h be the equation of*

$$-\Delta_h u_h = f_I \ \text{ at } \Omega_h \backslash \Gamma_h, \quad u_h = g_I \ \text{ at } \Gamma_h. \tag{12}$$

Then

$$\|u_h\|_{\infty,\Omega_h} \leq \frac{1}{8}\|f_I\|_{\infty,\Omega_h\backslash\Gamma_h} + \|g_I\|_{\Gamma_h,\infty}. \tag{13}$$

Proof. We introduce the comparison function

$$\phi = \frac{1}{4}\Big[(x-\frac{1}{2})^2 + (y-\frac{1}{2})^2\Big],$$

which satisfies $\Delta_h \phi_I = 1$ at $\Omega_h \backslash \Gamma_h$ and $0 \leq \phi \leq 1/8$. Set $M = \|f_I\|_{\infty,\Omega_h\backslash\Gamma_h}$. Then

$$\Delta_h(u_h + M\phi_I) = \Delta_h u_h + M \geq 0,$$

so

$$\max_{\Omega_h} u_h \leq \max_{\Omega_h}(u_h + M\phi_I) \leq \max_{\Gamma_h}(u_h + M\phi_I) \leq \max_{\Gamma_h} g_I + \frac{1}{8}M.$$

Thus u_h is bounded above by the right-hand side of (13). A similar argument applies to $-u_h$ giving the theorem. $\square$

Corollary 3.3. *Let u be the solution of the Dirichlet problem (4) and u_h the solution of the discrete problem (12). Then*

$$\|u_I - u_h\|_{\infty,\Omega_h} \leq \frac{1}{8}\|\Delta_h u_I - (\Delta u)_I\|_{\infty,\Omega_h\backslash\Gamma_h}.$$

The next step is to study the consistence error $\|\Delta_h u_I - (\Delta u)_I\|_{h,\infty}$. The following Lemma can be easily proved by Taylor expansion.

Lemma 3.4. *If $u \in \mathcal{C}^4(\Omega)$, then*

$$\|\Delta_h u_I - (\Delta u)_I\|_{\infty,\Omega_h\backslash\Gamma_h} \leq \frac{h^2}{6}\max\{\|\frac{\partial^4 u}{\partial x^4}\|_{\infty,\Omega_h\backslash\Gamma_h}, \|\frac{\partial^4 u}{\partial y^4}\|_{\infty,\Omega_h\backslash\Gamma_h}\}.$$

We summarize the convergence results on the finite difference methods in the following theorem.

Theorem 3.5. *Let u be the solution of the Dirichlet problem (4) and u_h the solution of the discrete problem (12). If $u \in \mathcal{C}^4(\Omega)$, then*

$$\|u_I - u_h\|_{\infty,\Omega_h} \leq Ch^2,$$

with constant

$$C = \frac{1}{48}\max\{\|\frac{\partial^4 u}{\partial x^4}\|_\infty, \|\frac{\partial^4 u}{\partial y^4}\|_\infty\}.$$

In practice, the second order of convergence can be observed even the solution u is less smooth than $\mathcal{C}^4(\Omega)$, i.e. the requirement $u \in \mathcal{C}^4(\Omega)$. This restriction comes from the point-wise estimate. In finite element method, we shall use integral norms to find the right setting of function spaces.

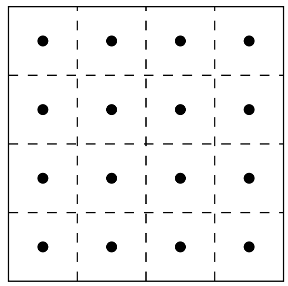

FIGURE 1. A cell centered uniform grid

4. CELL CENTERED FINITE DIFFERENCE METHODS

In some applications, notable the computational fluid dynamics (CFD), the Poisson equation is solved on slightly different grids. In this section, we consider FDM for the Poisson equation at cell centers; see Fig 4.

At interior nodes, the standard $(4,-1,-1,-1,-1)$ but boundary conditions will be treated differently. The distance in axis direction between interior nodes is still h but the near boundary nodes (centers of the cells touching boundary) is $h/2$ away from the boundary. One can then easily verify that for Neumann boundary condition, the stencil for near boundary nodes is $(3,-1,-1,-1)$ and for corner cells $(2,-1,-1)$. Of course the boundary condition g should be evaluated and moved to the right hand side.

The Dirichlet boundary condition is more subtle for cell centered difference. We can still introduce the ghost grid points and use standard $(4,-1,-1,-1)$ stencil for near boundary nodes. But no grid points are on the boundary. The ghost value can be eliminated by linear extrapolation, i.e, requiring $(u_{0,j}+u_{1,j})/2 = g(0,y_j) := g_{1/2,j}$.

$$\frac{5u_{1,j}-u_{2,j}-u_{1,j-1}-u_{1,j+1}}{h^2} = f_{1,j} + \frac{2g_{1/2,j}}{h^2}. \tag{14}$$

The stencil will be $(5,-1,-1,-1,-2)$ for near boundary nodes and $(6,-1,-1,-2,-2)$ for corner nodes. The symmetry of the corresponding matrix is still preserved.

However, this treatment is of low order (see Exercise 3). To obtain a better truncation error, we can use the quadratic extrapolation, that is, use $u_{1/2,j}, u_{1,j}, u_{2,j}$ to fit a quadratic function and evaluate at $u_{0,j}$, we get $u_{0,j} = -2u_{1,j} + \frac{1}{3}u_{2,j} + \frac{8}{3}u_{1/2,j}$, and obtain the modified boundary scheme should be:

$$\frac{6u_{1,j}-\frac{4}{3}u_{2,j}-u_{1,j-1}-u_{1,j+1}}{h^2} = f_{1,j} + \frac{\frac{8}{3}g_{1/2,j}}{h^2}. \tag{15}$$

We denote the near boundary stencil by $(6,-\frac{4}{3},-1,-1,-\frac{8}{3})$. The quadratic extrapolation will lead to a better rate of convergence since the truncation error is improved. The disadvantage of this treatment is that the symmetry of the matrix is destroyed.

For the Poisson equation, there is another way to keep the second order truncation error and symmetry. For simplicity, let us consider the homogenous Dirichlet boundary condition, i.e., $u|_{\partial\Omega} = 0$. Then the tangential derivatives along the boundary is vanished, in particular, $\partial_t^2 u = 0$. Assume the equation $-\Delta u = f$ holds also on the boundary condition. Note that on the boundary, the Δ operator can be written as $\partial_t^2 + \partial_n^2$. We then get $\partial_n^2 u = \pm f$ on $\partial\Omega$. The sign is determined by if the norm direction is the same as the axis direction. Then we can use $u_1, u_{1/2} = 0$ and $\partial_n^2 u = f$ to fit a quadratic function and extrapolate to get an equation for the ghost point

$$u_{1,j} + u_{0,j} = \frac{h^2}{4} f_{1/2,j}$$

and modify the boundary stencil as

$$\frac{5u_{1,j} - u_{2,j} - u_{1,j-1} - u_{1,j+1}}{h^2} = f_{1,j} + \frac{1}{4} f_{1/2,j}. \tag{16}$$

5. Exercises

(1) Prove the following properties of the matrix A formed in the finite difference methods for Poisson equation with Dirichlet boundary condition:
  (a) it is symmetric: $a_{ij} = a_{ji}$;
  (b) it is diagonally dominant: $a_{ii} \geq -\sum_{j=1,j\neq i}^{N} a_{ij}$;
  (c) it is positive definite: $u^t A u \geq 0$ for any $u \in \mathbb{R}^N$ and $u^t A u = 0$ if and only if $u = 0$.

(2) Let us consider the finite difference discritization of Poisson equation with Neumann boundary condition.
  (a) Write out the 9×9 matrix A for $h = 1/2$.
  (b) Prove that in general the matrix corresponding to Neumann boundary condition is only semi-positive definite.
  (c) Show that the kernel of A consists of constant vectors: $Au = 0$ if and only if $u = c$.

(3) Check the truncation error of schemes (14), (15) and (16) for different treatments of Dirichlet boundary condition in the cell centered finite difference methods.