Finite difference method: A glance at discretizing PDEs

We know from Calculus that $f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$.

PDEs quickly become impossibly difficult to approach with exact solution techniques.

It is common therefore to proceed numerically. One approach is to discretize the problem.

For instance. We could use $f'(x) \approx \frac{1}{h} [f(x+h) - f(x)]$ to replace f'(x) with the finite difference on the RHS.

Such approximate methods are called finite difference methods.

Finite difference methods are a common approach to numerically solving PDEs.

The ODE or PDE translates into a (sparse) system of linear equations which is then solved using Linear Algebra.

Example 169.

- $f'(x) \approx \frac{1}{h} [f(x+h) f(x)]$ is a forward difference for f'(x).
- $f'(x) \approx \frac{1}{h} [f(x) f(x-h)]$ is a backward difference for f'(x).
- $f'(x) \approx \frac{1}{2h} [f(x+h) f(x-h)]$ is a central difference for f'(x). Note that this is the average of the forward and the backward difference. The calculations below show that the central difference performs better as an approximation of f'(x).

Comment. Recall that power series f(x) have the Taylor expansion $f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!} (x - x_0)^n$.

Equivalently, $f(x+h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!} h^n = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O(h^4).$ It follows that $\frac{1}{h} [f(x+h) - f(x)] = f'(x) + \boxed{\frac{h}{2} f''(x) + O(h^2)} = f'(x) + \boxed{O(h)}.$

The error is of order O(h). On the other hand, combining

$$\begin{split} f(x+h) &= f(x) + h \, f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O(h^4), \\ f(x-h) &= f(x) - h \, f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + O(h^4), \end{split}$$

it follows that

$$\frac{1}{2h}[f(x+h) - f(x-h)] = f'(x) + \boxed{\frac{h^2}{6}f'''(x) + O(h^3)} = f'(x) + \boxed{O(h^2)}.$$

The error is of order $O(h^2)$.

Comment. An error of order h^2 means that if we cut h by a factor of, say, $\frac{1}{10}$, then we expect the error to be cut by a factor of $\frac{1}{10^2} = \frac{1}{100}$.

Example 170. Find a central difference for f''(x).

Solution. Adding the two expansions for f(x+h) and f(x-h) to kill the f'(x) terms, and subtracting 2f(x), we find that

$$\frac{1}{h^2}[f(x+h) - 2f(x) + f(x-h)] = f''(x) + \boxed{\frac{h^2}{12}f^{(4)}(x) + O(h^3)} = f''(x) + \boxed{O(h^2)}$$

The error is of order 2.

Alternatively. If we iterate the approximation $f'(x) \approx \frac{1}{2h} [f(x+h) - f(x-h)]$ (in the second step, we apply it with x replaced by $x \pm h$), we obtain

$$f''(x) \approx \frac{1}{2h} [f'(x+h) - f'(x-h)] \approx \frac{1}{4h^2} [f(x+2h) - 2f(x) + f(x-2h)],$$

which is the same as what we found above, just with h replaced by 2h.

Example 171. (discretizing Δ) Use the above central difference approximation for second derivatives to derive a finite difference for $\Delta u = u_{xx} + u_{yy}$ in 2D.

Solution.

$$\begin{aligned} u_{xx} + u_{yy} &\approx \frac{1}{h^2} [u(x+h,y) - 2u(x,y) + u(x-h,y)] + \frac{1}{h^2} [u(x,y+h) - 2u(x,y) + u(x,y-h)] \\ &= \frac{1}{h^2} [u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h) - 4u(x,y)] \end{aligned}$$

Notation. This finite difference is typically represented as $\frac{1}{h^2}\begin{bmatrix} 1\\ 1 & -4 & 1\\ 1 & \end{bmatrix}$, the five-point stencil.

Comment. Recall that solutions to $\Delta u = 0$ are supposed to describe steady-state temperature distributions. We can see from our discretization that this is reasonable. Namely, $\Delta u = 0$ becomes approximately equivalent to

$$u(x, y) = \frac{1}{4}(u(x+h, y) + u(x-h, y) + u(x, y+h) + u(x, y-h))$$

In other words, the temperature u(x, y) at a point (x, y) should be the average of the temperatures of its four "neighbors" u(x+h, y) (right), u(x-h, y) (left), u(x, y+h) (top), u(x, y-h) (bottom).

Comment. Think about how to use this finite difference to numerically solve the corresponding Dirichlet problem by discretizing (one equation per lattice point).

Advanced comment. If $\Delta u = 0$ then, when discretizing, the center point has the average value of the four points adjacent to it. This leads to the maximum principle: if $\Delta u = 0$ on a region R, then the maximum (and, likewise, minimum) value of u must occur at a boundary point of R.

Example 172. Discretize the following Dirichlet problem:

$$u_{xx} + u_{yy} = 0$$
 (PDE)
 $u(x, 0) = 2$
 $u(x, 2) = 3$
 $u(0, y) = 0$
 $u(1, y) = 0$
(BC)

Use a step size of $h = \frac{1}{3}$.

Comment. Note that, for the Dirichlet problem as well as for our discretization, it doesn't matter that the boundary conditions aren't well-defined at the corners.

Solution. Note that our rectangle has side lengths 1 (in x direction) and 2 (in y direction). With a step size of $h = \frac{1}{3}$ we therefore get $4 \cdot 7$ lattice points, namely the points

$$u_{m,n} = u(mh, nh), \quad m \in \{0, 1, 2, 3\}, n \in \{0, 1, ..., 6\}.$$

Further note that the boundary conditions determine the values of $u_{m,n}$ if m = 0 or m = 3 as well as if n = 0 or n = 6. This leaves $2 \cdot 5 = 10$ points at which we need to determine the value of $u_{m,n}$.

Next, we approximate $u_{xx} + u_{yy}$ by $\frac{1}{h^2}[u(x+h, y) + u(x-h, y) + u(x, y+h) + u(x, y-h) - 4u(x, y)]$ (see previous example for how we obtained this finite difference approximation). Note that, if $u(x, y) = u_{m,n}$ is one of our lattice points, then the other four terms in the finite difference are lattice points as well; for instance, $u(x+h, y) = u_{m+1,n}$. The equation $u_{xx} + u_{yy} = 0$ therefore translates into

$$u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{m,n} = 0$$

Spelling out these equation for each $m \in \{1, 2\}$ and $n \in \{1, 2, ..., 5\}$, we get 10 (linear) equations for our 10 unknown values. For instance, here are the equations for (m, n) = (1, 1), (1, 2) as well as (2, 5):

$$u_{2,1} + u_{0,1} + u_{1,2} + u_{1,0} - 4u_{1,1} = 0$$

$$u_{2,2} + u_{0,2} + u_{1,3} + u_{1,1} - 4u_{1,2} = 0$$

$$\vdots$$

$$u_{3,5} + u_{1,5} + u_{2,6} + u_{2,4} - 4u_{2,5} = 0$$

In matrix-vector form, these linear equations take the form:

$$\begin{bmatrix} -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \vdots & & & & \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ u_{1,4} \\ u_{1,5} \\ u_{2,1} \\ u_{2,2} \\ u_{2,3} \\ u_{2,4} \\ u_{2,5} \end{bmatrix} = \begin{bmatrix} -2 \\ 0 \\ \vdots \\ -3 \end{bmatrix}$$

Solving this system, we find $u_{1,1} \approx 0.7847$, $u_{1,2} \approx 0.3542$, ..., $u_{2,5} \approx 1.1597$.

For comparison, the corresponding exact values are $u\left(\frac{1}{3},\frac{1}{3}\right) \approx 0.7872$, $u\left(\frac{1}{3},\frac{2}{3}\right) \approx 0.3209$, ..., $u\left(\frac{2}{3},\frac{5}{3}\right) \approx 1.1679$. These were computed from the exact formula

$$u(x,y) = \sum_{\substack{n=1\\n \text{ odd}}}^{\infty} \frac{4}{\pi n} \frac{\sin(\pi n x)}{1 - e^{4\pi n}} [2(e^{\pi n y} - e^{-\pi n(y-4)}) + 3(e^{\pi n(2-y)} - e^{\pi n(2+y)})],$$

which we will derive soon.

Armin Straub straub@southalabama.edu The three plots below visualize the discretized solution with $h = \frac{1}{3}$ from Example 172, the exact solution, as well as the discretized solution with $h = \frac{1}{20}$.



Comment. The first plot looks a bit overly rough because we chose not to interpolate the values. As we showed above, the approximate values at the ten lattice points are actually pretty decent for such a large step size. Warning. The resulting linear systems quickly become very large. For instance, if we use a step size of $h = \frac{1}{100}$, then we need to determine roughly $100 \cdot 200 = 20,000$ (99 \cdot 199 to be exact) values $u_{m,n}$. The corresponding matrix M will have about $20,000^2 = 400,000,000$ entries, which is already challenging for a weak machine if we use generic linear algebra software. At this point it is important to realize that most entries of the matrix M are 0. Such matrices are called **sparse** and there are efficient algorithms for solving systems involving such matrices.

Example 173. Discretize the following Dirichlet problem:

$$u_{xx} + u_{yy} = 0 \text{ (PDE)}$$

$$u(x, 0) = 2$$

$$u(x, 1) = 3$$

$$u(0, y) = 1$$

$$u(2, y) = 4$$

(BC)

Use a step size of $h = \frac{1}{2}$.

Solution. Note that our rectangle has side lengths 2 (in x direction) and 1 (in y direction). With a step size of $h = \frac{1}{2}$ we therefore get $5 \cdot 3$ lattice points, namely the points

$$u_{m,n} = u(mh, nh), \quad m \in \{0, 1, 2, 3, 4\}, \ n \in \{0, 1, 2\}.$$

Further note that the boundary conditions determine the values of $u_{m,n}$ if m = 0 or m = 4 as well as if n = 0 or n = 2. This leaves $3 \cdot 1 = 3$ points at which we need to determine the value of $u_{m,n}$.

If we approximate $u_{xx} + u_{yy}$ by $\frac{1}{h^2}[u(x+h, y) + u(x-h, y) + u(x, y+h) + u(x, y-h) - 4u(x, y)]$ then, in terms of our lattice points, the equation $u_{xx} + u_{yy} = 0$ translates into

$$u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{m,n} = 0$$

Spelling out these equation for each $m \in \{1, 2, 3\}$ and n = 1, we get 3 equations for our 3 unknown values:

$$\begin{array}{rcl} u_{2,1} + \underbrace{u_{0,1}}_{=1} + \underbrace{u_{1,2}}_{=3} + \underbrace{u_{1,0}}_{=2} - 4u_{1,1} &=& 0 \\ u_{3,1} + u_{1,1} + \underbrace{u_{2,2}}_{=3} + \underbrace{u_{2,0}}_{=2} - 4u_{2,1} &=& 0 \\ \underbrace{u_{4,1}}_{=4} + u_{2,1} + \underbrace{u_{3,2}}_{=3} + \underbrace{u_{3,0}}_{=2} - 4u_{3,1} &=& 0 \\ \end{array}$$

In matrix-vector form, these linear equations take the form:

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{2,1} \\ u_{3,1} \end{bmatrix} = \begin{bmatrix} -6 \\ -5 \\ -9 \end{bmatrix}$$