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 167.

- $f'(x) \approx \frac{1}{h}[f(x+h) - f(x)]$ 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, $f(x+h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!} h^n = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O(h^4)$. 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 $\boxed{\text{error}}$ is of order $O(h)$. On the other hand, combining

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

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 $\boxed{\text{error}}$ 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 168. 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 $\boxed{\text{error}}$ 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 169. (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 170. Discretize the following Dirichlet problem:

$$\begin{aligned} u_{xx} + u_{yy} &= 0 \quad \text{(PDE)} \\ u(x,0) &= 2 \\ u(x,2) &= 3 \\ u(0,y) &= 0 \\ u(1,y) &= 0 \end{aligned} \quad \text{(BC)}$$

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

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

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 $n \in \{1,2,\ldots,5\}$, 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 $(2,5)$:

$$\begin{aligned} u_{2,1} + \underbrace{u_{0,1}}_{=0} + u_{1,2} + \underbrace{u_{1,0}}_{=2} - 4u_{1,1} &= 0 \\ u_{2,2} + \underbrace{u_{0,2}}_{=0} + u_{1,3} + u_{1,1} - 4u_{1,2} &= 0 \\ &\vdots \\ \underbrace{u_{3,5}}_{=0} + u_{1,5} + \underbrace{u_{2,6}}_{=3} + u_{2,4} - 4u_{2,5} &= 0 \end{aligned}$$

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

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

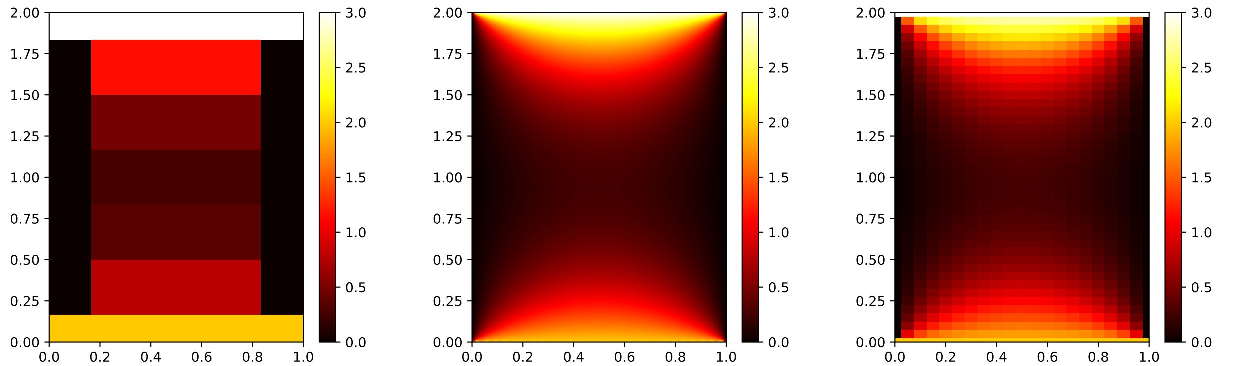
Solving this system, we find $u_{1,1} \approx 0.7847$, $u_{1,2} \approx 0.3542$, ..., $u_{2,5} \approx 1.1597$.

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.

The three plots below visualize the discretized solution with $h = \frac{1}{3}$ from Example 170, 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 171. Discretize the following Dirichlet problem:

$$\begin{aligned} u_{xx} + u_{yy} &= 0 \quad \text{(PDE)} \\ u(x,0) &= 2 \\ u(x,1) &= 3 \\ u(0,y) &= 1 \\ u(2,y) &= 4 \end{aligned} \qquad \text{(BC)}$$

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:

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

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

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