A glance at discretizing PDEs

One of the most important partial differential equations is the following equation which, for instance, models the steady-state temperature $u(x,y)$ of a region in two-dimensional space.

(Laplace equation, 2D)

$$u_{xx}+u_{yy}=0$$

Notation. Here, for instance, $u_{xx}=\frac{\partial^2}{\partial x^2}u(x,y)$ is used to denote two partial derivatives with respect to x.

The Laplace equation is often written as $\Delta u=0$, where $\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}$ is the Laplace operator you may know from Calculus III.

The Laplacian Δu is also often written as $\Delta u=\nabla^2 u$. The operator $\nabla=(\partial/\partial x,\partial/\partial y)$ is pronounced "nabla" (Greek for a certain harp) or "del" (Persian for heart), and ∇^2 is short for the inner product $\nabla\cdot\nabla$.

Higher dimensions. Likewise, the Laplace equation in three dimensions is $\Delta u=0$ with $\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$.

Comment. The Laplace equation is so important that its solutions have their own name: **harmonic functions**.

It is also known as the **potential equation** and is satisfied by electric/gravitational potential functions.

Recall from Calculus III (if you have taken that class) that the gradient of a scalar function $f(x,y)$ is the vector field $\boldsymbol{F}=\operatorname{grad} f=\nabla f=\begin{bmatrix} f_x(x,y) \\ f_y(x,y) \end{bmatrix}$. One says that $\boldsymbol{F}$ is a **gradient field** and f is a **potential function** for $\boldsymbol{F}$ (for instance, $\boldsymbol{F}$ could be a gravitational field with gravitational potential f).

One way to describe a unique solution to the Laplace equation within a region is by specifying the values of $u(x,y)$ along the boundary of that region.

This is particularly natural for steady-state temperatures profiles of a region R. The Laplace equation governs how temperature behaves inside the region but we need to also prescribe the temperature on the boundary.

The PDE with such a boundary condition is called a Dirichlet problem:

(Dirichlet problem)

$u_{xx}+u_{yy}=0$ within region R

$u(x,y)=f(x,y)$ on boundary of R

In general. A Dirichlet problem consists of a PDE, that needs to hold within a region R, and prescribed values on the boundary of that region ("Dirichlet boundary conditions").

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Discretizing the Laplace operator

Recall from Example 117 that the following central difference is an order 2 approximation of $f''(x)$.

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

Example 153. (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 154. Discretize the following Dirichlet problem:

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

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

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

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 $(2,5)$:

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

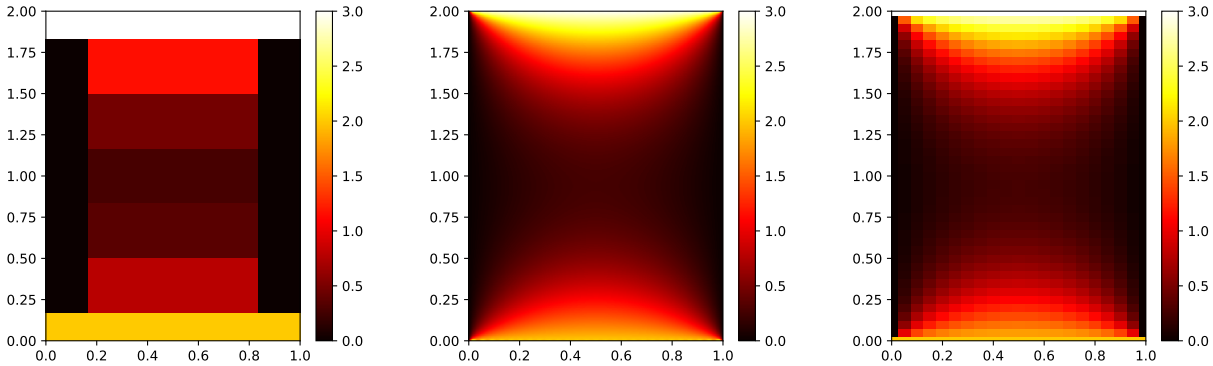
In matrix-vector form, these linear equations take the form:

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

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 $u\left(\frac{1}{3},\frac{1}{3}\right)\approx 0.7872$, $u\left(\frac{1}{3},\frac{2}{3}\right)\approx 0.3209$, ..., $u\left(\frac{2}{3},\frac{5}{3}\right)\approx 1.1679$.

The three plots below visualize the discretized solution with $h=\frac{1}{3}$ from Example 154, 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 155. Discretize the following Dirichlet problem:

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

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:

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