Project 1

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1 Introduction

Efficiently solving differential equations is essential to many problems in computational science. One particularly frequent class of differential equations are linear second-order differential equations, which can be written as

$$\frac{d^2y}{dx^2} + k(x)y = f(x) \tag{1}$$

for some source function $f(x)$ and a real function $k(x)$.

One example of an equation of this form is found in classical electrostatics. There, the electric field of a point charge can be found using Poisson's equation:

$$\nabla^2\Phi(\mathbf{r}) = -4\pi\rho(\mathbf{r}) \tag{2}$$

where $\rho(\mathbf{r})$ is the charge distribution. Assuming spherical symmetry, this becomes a one-dimensional equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = -4\pi\rho(r)$$

which can be written as

$$\frac{d^2\phi}{dr^2} = -4\pi r\rho(r)$$

by letting $\Phi(r) = \phi(r)/r$. This is now a linear second-order differential equation of the form shown in (1) where $k(r) = 0$ and $f(r) = -4\pi r\rho(r)$. To simplify things further, let $r \to x$ and $\phi \to u$, and then define $f(x) = -4\pi x\rho(x)$. Then our equation becomes

$$-u''(x) = f(x)$$

Equations of this form can occasionally be solved analytically, but in general they must be solved using numerical methods.

2 Numerical algorithm

To make the problem more concrete, we will be solving the equation

$$-u''(x) = f(x) \tag{3}$$

on the domain $x \in [0, 1]$ with Dirichlet boundary conditions $u(0) = u(1) = 0$.

The second derivative can be found using the second-order finite difference relation

$$u''(x) \approx \frac{u(x+h) + u(x-h) - 2u(x)}{h^2} + O(h^2) \tag{4}$$

for some small step size h. Plugging this relation into (3) produces the equation

$$-\frac{u(x+h) + u(x-h) - 2u(x)}{h^2} = f(x). \tag{5}$$

Next, we discretize the problem by creating a mesh of step size h between the lower and upper boundaries. This is conceptually the same as representing the functions $u(x)$ and $f(x)$ as vectors u_i and f_i. Thus, we can write

$$-\frac{u_{i+1} + u_{i-1} - 2u_i}{h^2} = f_i, \quad i = 1, \ldots, n. \tag{6}$$

Thinking of u and f as vectors, this can be interpreted as taking the $(i+1)$-th element of u, the $(i-1)$-th element of u, and so on. This leads to a natural interpretation of this equation in terms of a set of linear equations

$$\begin{pmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & \ddots & \ddots & & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_n \end{pmatrix} \tag{7}$$

where $w_i \equiv h^2 f_i$, and all elements not shown in the matrix are taken to be zero. This is a *tridiagonal* matrix, meaning it has elements only on the primary diagonal and on the diagonals above and below it.