COMPUTATIONAL PDE LECTURE 7

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1. Outline of today

- Discrete maximum principle and stability
- Handling Neumann boundary conditions

2. Neumann Boundary Conditions

How would we implement a Neumann BC for the following problem?

$$\begin{cases} -u''(x) & = f(x) \\ u'(0) = g_\ell \\ u(1) = u_r \end{cases} \tag{1}$$

One option would be to have the discretized equation use a forward difference:

$$\frac{U^h(x_1) - U^h(x_0)}{h} = g_\ell$$

The issue with this approximation is that the truncation error is for some $C > 0$:

$$\left| \frac{u(x_1) - u(x_0)}{h} \right| = Ch \max_{z \in [0,1]} |u''(z)|,$$

which means we'd potentially have a reduced convergence rate.

2.1. **Trick: Ghost point.**

The neat trick is to use a technique called a ghost point, which utilizes a centered finite difference at 0:

$$\frac{U^h(x_1) - U^h(x_{-1})}{2h} = g_\ell$$

where $x_{-1} = -h$. This centered difference does not give us a useable equation, but we can use the differential equation approximation to write

$$\frac{-U^h(x_1) + 2U^h(x_0) - U^h(x_{-1})}{h^2} = f(x_0)$$

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Since $U^h(x_{-1}) = U^h(x_1) - 2hg_\ell$, we have

$$\frac{2U^h(x_0) - 2U^h(x_1)}{h^2} = f(x_0) - \frac{2g_\ell}{h}$$

and the resulting linear system is:

$$\underbrace{\begin{pmatrix} \frac{2}{h^2} & \frac{-2}{h^2} & \cdots & & \\ -\frac{1}{h^2} & \frac{2}{h^2} & -\frac{1}{h^2} & 0 & \cdots \\ & \ddots & \ddots & \ddots & \\ \cdots & 0 & -\frac{1}{h^2} & \frac{2}{h^2} & -\frac{1}{h^2} \\ & & \cdots & 0 & 1 \end{pmatrix}}_{=:\mathbf{A}^h} \underbrace{\begin{pmatrix} U^h(x_0) \\ U^h(x_1) \\ \vdots \\ U^h(x_{N-1}) \\ U^h(x_N) \end{pmatrix}}_{=:\mathbf{U}^h} = \underbrace{\begin{pmatrix} f(x_0) - \frac{2g_\ell}{h} \\ f(x_1) \\ \vdots \\ f(x_{N-1}) \\ u_r \end{pmatrix}}_{\mathbf{f}^h}. \tag{2}$$

Remark 2.1. Note that the matrix $\mathbf{A}^h$ is no longer symmetric. This can be fixed by multiplying

$$\frac{2U^h(x_0) - 2U^h(x_1)}{h^2} = f(x_0) - \frac{2g_\ell}{h}$$

by $\frac{1}{2}$ to get

$$\frac{U^h(x_0) - U^h(x_1)}{h^2} = \frac{1}{2} f(x_0) - \frac{g_\ell}{h}$$

and the matrix system is:

$$\underbrace{\begin{pmatrix} \frac{1}{h^2} & \frac{-1}{h^2} & \cdots & & \\ -\frac{1}{h^2} & \frac{2}{h^2} & -\frac{1}{h^2} & 0 & \cdots \\ & \ddots & \ddots & \ddots & \\ \cdots & 0 & -\frac{1}{h^2} & \frac{2}{h^2} & -\frac{1}{h^2} \\ & & \cdots & 0 & 1 \end{pmatrix}}_{=:\mathbf{A}^h} \underbrace{\begin{pmatrix} U^h(x_0) \\ U^h(x_1) \\ \vdots \\ U^h(x_{N-1}) \\ U^h(x_N) \end{pmatrix}}_{=:\mathbf{U}^h} = \underbrace{\begin{pmatrix} \frac{1}{2} f(x_0) - \frac{g_\ell}{h} \\ f(x_1) \\ \vdots \\ f(x_{N-1}) \\ u_r \end{pmatrix}}_{\mathbf{f}^h} \tag{3}$$

which is now symmetric.

2.2. **Another approach.** Another approach would be to discretize the Neumann BC with the following finite difference:

$$u'(x_0) \approx \frac{-3u(x_0) + 4u(x_1) - u(x_2)}{2h},$$

which you'll see in the HW satisfies:

$$u'(x_0) = \frac{-3u(x_0) + 4u(x_1) - u(x_2)}{2h} + O(h^2).$$

One drawback of this method is that you cannot make the resulting matrix $\mathbf{A}^h$ symmetric.

3. Variational Principle for Poisson's Equation

We now conclude with a variational principle for Poisson equation. Consider that the discrete $\mathbf{U}^h$ solves the following system of linear equations.

$$\mathbf{A}^h\mathbf{U}^h = \mathbf{f}^h$$

Observe that if

$$\mathbf{U}^h \text{ minimizes } \mathbf{v}^h \mapsto \frac{1}{2}{\mathbf{v}^h}^T\mathbf{A}^h\mathbf{v}^h - \mathbf{f}^h\mathbf{v}^h$$

then

$$\mathbf{A}^h\mathbf{U}^h = \mathbf{f}^h.$$

In fact we have an analogous result for $\mathbf{u}$ solving Poisson's equation.

Proposition 3.1. Suppose $u \in C^1[0,1]$ subject to $u(0) = u(1) = 0$ minimizes

$$E[w] = \int_\Omega \frac{1}{2}|w'(x)|^2 - f(x)w(x)dx$$

over all possible $w \in C^1[0,1]$ subject to $w(0) = w(1) = 0$, then u satisfies

$$\int_\Omega u'(x)v'(x)dx = \int_\Omega f(x)v(x)dx$$

for all $v \in C^1[0,1]$ subject to $v(0) = v(1) = 0$. As shown in the HW, this is the weak form of Poisson's equation:

$$\begin{cases} -u''(x) = f(x)x \in (0,1) \\ u(0) = u(1) = 0 \end{cases}$$

Proof. Let u minimize E and let $w^t = u + tv$, where $t > 0$ and $v \in C^1[0,1]$ subject to $v(0) = v(1) = 0$. Then $w^t \in C^1[0,1]$ and $w^t(0) = w^t(1) = 0$. Since u is a minimizer we have,

$$0 \leq E[w^t] - E[u] = E[u + tv] - E[u]$$

We now expand $E[u + tv]$:

$$\begin{aligned} E[u+tv] &= \int_\Omega \frac{1}{2}|u'(x) + tv'(x)|^2 - f(x)(u(x) + tv(x))dx \\ &= \int_\Omega \frac{1}{2}|u'(x)|^2 + \frac{t^2}{2}|v'(x)|^2 + tu'(x)v'(x) - f(x)(u(x) + tv(x))dx \end{aligned}$$

Subtracting $E[u]$ yields and dividing by t yields

$$\frac{E[u+tv] - E[u]}{t} = \int_\Omega \frac{t}{2}|v'(x)|^2 + u'(x)v'(x) - f(x)v(x)dx$$

Taking a limit as $t \to 0$ leads to

$$\int_\Omega u'(x)v'(x) - f(x)v(x)dx \geq 0$$

Repeating the argument for $w^t = u - tv$ also shows

$$\int_\Omega u'(x)v'(x) - f(x)v(x)dx \leq 0$$

Hence

$$\int_\Omega u'(x)v'(x) - f(x)v(x)dx = 0,$$

which is the weak form. □

The reverse direction is also true.

Proposition 3.2. Suppose $u \in C^1[0,1]$ satisfies

$$\int_\Omega u'(x)v'(x)dx = \int_\Omega f(x)v(x)dx$$

for all $v \in C^1[0,1]$ subject to $v(0) = v(1) = 0$. Then, u minimizes

$$E[w] = \int_\Omega \frac{1}{2}|w'(x)|^2 - f(x)w(x)dx$$

over all possible $w \in C^1[0,1]$ subject to $w(0) = w(1) = 0$.

Proof. Let $w \in C^1[0,1]$ subject to $w(0) = w(1) = 0$. Let u solve the weak form of Poisson's equation. We let $v = w - u$, which satisfies $v(0) = v(1) = 0$. Then,

$$\begin{aligned}
E[w] - E[u] =& E[u+v] - E[u] \\
= \int_\Omega \frac{1}{2}|u'(x)|^2 + \frac{1}{2}|v'(x)|^2 + u'(x)v'(x) - f(x)(u(x)+v(x))dx &- \int_\Omega \frac{1}{2}|u'(x)|^2 - f(x)u(x)dx \\
&= \int_\Omega \frac{1}{2}|v'(x)|^2 dx + \underbrace{\int_\Omega u'(x)v'(x) - f(x)v(x)dx}_{=0} \\
&= \int_\Omega \frac{1}{2}|v'(x)|^2 dx \geq 0
\end{aligned}$$

Hence, $E[w] \geq E[u]$ for all $w \in C^1[0,1]$ subject to $w(0) = w(1) = 0$. □

These variational principles work for much more general problems. For instance, minimizing the energy:

$$E[u] = \int_\Omega \frac{1}{2}|u'(x)|^2 + f(u(x))dx$$

leads to the following weak form:

$$\int_\Omega u'(x)v'(x) + f'(u(x))v(x)dx = 0,$$

and whose strong form is

$$-u''(x) + f'(u(x)) = 0.$$

In HW2, the PDE

$$-u''(x) + \frac{1}{\varepsilon^2}u(x)(u(x)^2 - 1) = 0$$

is a PDE corresponding to the energy:

$$\int_\Omega \frac{1}{2}|u'(x)|^2 + \frac{1}{\varepsilon^2}(u(x)^2 - 1)^2 dx$$