18.336/6.335 Fast Methods for Partial Differential and Integral Equations Spring 2013

February 21-, 2013

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4 Integral Equation Methods

4.1 The Exterior Problem

Once again, let us return to the Poisson Equation:

$$\Delta u = f, \quad x \in \Omega, \Omega \in \mathbb{R}^d, d = \{2, 3\}$$

However, unlike before, let us consider the exterior problem with no physical finite boundary. That is, there is no finite "box" enclosing the problem domain; instead we impose the following condition out at infinity:

$$\lim_{|x|\to\infty} u(x) = 0$$

The exterior problem is very common. Example applications include:

- Molecular Dynamics, where $\nabla u = E$ is the electric field, and the objective is to calculate the electrostatic forces between different molecules. There is no obvious boundary to the interaction.
- The Conservation Corrector in fluid calculations, where fluid velocity correction is ∇u and f comes from another part of the fluid code. The domain is a vast fluid body, e.g. the ocean.
- Electrochemistry: electrostatic potential $= u$. Charge is everywhere but yet again no definite boundary.

Consider using the finite difference approach to solve the exterior problem. The domain of interest for u is usually known in advance, but the solution domain and grid must be much larger in order to approximate the boundary out at infinity. Let K be the 1D Dirichlet boundary condition finite difference method matrix. The 2D case is $K \otimes I + I \otimes K$. The 3D case is $K \otimes I \otimes I + I \otimes K \otimes I + I \otimes I \otimes K$. As each kronecker product increases the dimension of the governing matrix by one exponent, it is very expensive indeed to expand the computation to approximate the radiation condition.

4.2 Introducing the Green's function

An alternative approach is to use integral equations. If $G(x-x')$ is defined such that $\int(\Delta_x G(x-x'))f(x')\,\mathrm{d}x' = f(x)$ then $\Delta_x G(x-x') = \delta(x-x')$. Let

$$u(x) \equiv \int_\Omega G(x-x')f(x')\,\mathrm{d}x', \quad x \in \Omega$$

then,

$$\Delta u = f, \quad x \in \Omega.$$

Informally, this definition can be written as:

$$\Delta G = \delta,$$

where δ is the Dirac delta generalized function.

The 2D Laplacian Green's function is the following:

$$G_{2D}(\boldsymbol{r}) = \frac{1}{2\pi} \ln |\boldsymbol{r}|$$

The 3D Laplacian Green's function is:

$$G_{3D}(\boldsymbol{r}) = \frac{1}{4\pi} \frac{1}{|\boldsymbol{r}|}.$$

In physics, the Green's function is known as the response due to a point charge; in electrical engineering it is known as the impulse response; in mathematics it is known as the fundamental solution. Regardless, we only want to know $u(x)$ given that $x \in \Omega_{important}$:

$$u(x) = \int_{\Omega_{important}} G(x - x') f(x') \, \mathrm{d}x'$$

Now we evaluate the integral numerically using quadrature:

$$u(x) \approx \sum_j W(x_j) G(x - x_j) f(x_j)$$

where x_j are quadrature points and W are quadrature weights. Standard quadrature is ineffective around $x = x'$. Assuming unit areas, we can defining box averages:

$$u_i = \int_{box,i} u(x') \, \mathrm{d}x'$$

and

$$f_i = \int_{box,i} f(x') \, \mathrm{d}x'$$

Substituting to the original equation:

$$\begin{aligned} u_{box,i} &= \int_{box,i} \int_{allboxes} G(x - x') f(x') \, \mathrm{d}x' \, \mathrm{d}x \\ &= \int_{box,i} \sum_j \int_{box,j} G(x - x') f(x') \, \mathrm{d}x' \, \mathrm{d}x \end{aligned}$$

Suppose we make the only approximation in this problem:

$$f(x)_{x \in box,j} \approx f_{box,j}$$

Then we can write

$$\begin{aligned} u_{box,i} &= \int_{box,i} \sum_j \left(\int_{box,j} G(x - x') \, \mathrm{d}x' \right) f_{box,j} \, \mathrm{d}x \\ &= \sum_j f_{box,j} \int_{box,i} \int_{box,j} G(x - x') \, \mathrm{d}x' \, \mathrm{d}x \end{aligned}$$

When discretized we can write:

$$u_{box} = \overline{\overline{G}} f_{box}$$

where the matrix $\overline{\overline{G}}$ is Toeplitz, but not circulant:

$$\begin{bmatrix} u_{box,1} \\ \\ \\ u_{box,n} \end{bmatrix} = \begin{bmatrix} g_0 & g_{-1} & g_{-2} & \cdots & g_{-n} \\ g_1 & g_0 & g_{-1} & \ddots & \vdots \\ g_2 & g_1 & g_0 & \ddots & g_{-2} \\ \vdots & \ddots & \ddots & \ddots & g_{-1} \\ g_n & \cdots & g_2 & g_1 & g_0 \end{bmatrix} \begin{bmatrix} f_{box,1} \\ \\ \\ f_{box,n} \end{bmatrix}$$

We can make $\overline{\overline{G}}$ circulant by embedding it within a bigger matrix of $2n-1$ by $2n-1$.