Discretizing the Laplacian on Radial Functions

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Let u be a radial function on $B_a = \{x \in \mathbb{R}^n : |x| < a\}$,

$$u(x) = f(r), \quad r = |x|. \tag{1}$$

Then the Laplacian of u is given by

$$\Delta u(x) = f''(r) + \frac{n-1}{r} f'(r). \tag{2}$$

The fact that the coefficient $(n-1)/r$ of $f'(r)$ blows up as $r \searrow 0$ can be inconvenient. We examine here how to discretize Δu, in a fashion that avoids the singular behavior while retaining the one dimensional character.

To start, we recall the centered difference discretization, given as follows. Fix a mesh size h. Then

$$\frac{h^2}{2} \Delta_h u(x) = \frac{1}{2} \sum_{j=1}^{n} \big\{ u(x + he_j) + u(x - he_j) \big\} - nu(x), \tag{3}$$

where $\{e_1, \dots, e_n\}$ is the standard basis of $\mathbb{R}^n$. Using (1), we get

$$\frac{h^2}{2} \Delta_h f(r) = \frac{1}{2} \big[f(r+h) + f(r-h) \big] + (n-1) f\big(\sqrt{r^2 + h^2}\big) - nf(r). \tag{4}$$

Let us take $h = a/N$, for some (large) integer N. Our discrete representation of $f(r)$ will be

$$f_j = f(jh), \quad 0 \le j \le N, \tag{5}$$

and it is natural to set $f_{-1} = f_1$. Then the discrete representation of $\Delta_h f$ is G_j, satisfying

$$\frac{h^2}{2} G_j = \frac{1}{2} \big[f_{j+1} + f_{j-1} \big] + (n-1)\varphi_j - nf_j, \quad 0 \le j \le N-1, \tag{6}$$

where

$$\varphi_j = f\big(h\sqrt{j^2+1}\big) = f(jh + \xi_j), \tag{7}$$

with

$$\frac{\xi_j}{h} = \sqrt{j^2+1} - j = \frac{1}{\sqrt{j^2+1} + j}. \tag{8}$$

Clearly

$$\varphi_0 = f_1. \tag{9}$$

For $1 \leq j \leq N-1$, we find φ_j by *interpolating* f_{j-1}, f_j, and f_{j+1}. We set

$$\varphi_j = a_{-1}(\xi_j) f_{j-1} + a_0(\xi_j) f_j + a_1(\xi_j) f_{j+1}. \tag{10}$$

In detail, if we freeze j and set $F(\xi) = f(jh + \xi)$, with $0 < \xi < h$, then we make expansions

$$\begin{aligned} F(\xi) &= a_{-1}(\xi)F(-h) + a_0(\xi)F(0) + a_1(\xi)F(h) \\ &= a_{-1}(\xi)\Big(F(0) - F'(0)h + \frac{1}{2}F''(0)h^2 + \cdots\Big) + a_0(\xi)F(0) \\ &\quad + a_1(\xi)\Big(F(0) + F'(0)h + \frac{1}{2}F''(0)h^2 + \cdots\Big), \end{aligned} \tag{11}$$

and neglect higher powers of h, to write

$$\begin{aligned} F(\xi) = {} & \Big(a_{-1}(\xi) + a_0(\xi) + a_1(\xi)\Big)F(0) \\ & + \Big(a_1(\xi) - a_{-1}(\xi)\Big)F'(0)h \\ & + \frac{1}{2}\Big(a_1(\xi) + a_{-1}(\xi)\Big)F''(0)h^2. \end{aligned} \tag{12}$$

Comparison with

$$F(\xi) = F(0) + F'(0)\xi + \frac{1}{2}F''(0)\xi^2 \tag{13}$$

gives

$$\begin{aligned} a_1(\xi) + a_0(\xi) + a_{-1}(\xi) &= 1, \\ a_1(\xi) \qquad\quad - a_{-1}(\xi) &= \frac{\xi}{h}, \\ a_1(\xi) \qquad\quad + a_{-1}(\xi) &= \Big(\frac{\xi}{h}\Big)^2, \end{aligned} \tag{14}$$

hence

$$\begin{aligned} a_1(\xi) &= \frac{1}{2}\,\frac{\xi}{h}\Big(1 + \frac{\xi}{h}\Big), \\ a_{-1}(\xi) &= -\frac{1}{2}\,\frac{\xi}{h}\Big(1 - \frac{\xi}{h}\Big), \\ a_0(\xi) &= 1 - \Big(\frac{\xi}{h}\Big)^2. \end{aligned} \tag{15}$$

We plug (8) into (15) to get $a_\nu(\xi_j),\ \nu=-1,0,1$, and then use (10) to compute φ_j, for $1\le j\le N-1$ (and (9) for $j=0$). This then goes into the formula (6) for the discretized Laplacian, except at $j=N$.

Discretizing Δu at $j=N$, i.e., at the boundary of the ball B_a, requires a different formula. But this is well away from the singularity $r=0$, so one can take some method of discretizing (2). In fact, to numerically solve $\partial u/\partial t=\Delta u$ on $(0,1]\times B_a$, for $u(t,x)=f(t,|x|)$, with boundary condition $u(t,x)=0$ when $|x|=a$, we may not need to evaluate G_j at $j=N$, since for each t, $f_N=0$.

For more detail on G_j for $0\le j\le N-1$, we have

$$\frac{h^2}{2}G_j=\frac{1}{2}f_{j+1}+\frac{1}{2}f_{j-1}-f_j+(n-1)(\varphi_j-f_j), \tag{16}$$

and, with

$$\gamma_j=\frac{1}{\sqrt{j^2+1}+j}, \tag{17}$$

we have

$$\varphi_j-f_j=\frac{1}{2}\gamma_j(f_{j+1}-f_{j-1})+\gamma_j^2\Big(\frac{1}{2}f_{j+1}+\frac{1}{2}f_{j-1}-f_j\Big), \tag{18}$$

so

$$\begin{aligned}\frac{h^2}{2}G_j&=\big(1+(n-1)\gamma_j^2\big)\Big(\frac{1}{2}f_{j+1}+\frac{1}{2}f_{j-1}-f_j\Big)\\&\quad+\frac{n-1}{2}\gamma_j(f_{j+1}-f_{j-1}),\end{aligned} \tag{19}$$

hence, for $j\ge 1$,

$$\begin{aligned}G_j&=\big(1+(n-1)\gamma_j^2\big)\frac{1}{h^2}(f_{j+1}+f_{j-1}-2f_j)\\&\quad+\frac{n-1}{r_j}(2j\gamma_j)\frac{f_{j+1}-f_{j-1}}{2h},\end{aligned} \tag{20}$$

with

$$r_j=jh, \tag{21}$$

while

$$G_0=n\frac{f_1+f_{-1}-2f_0}{h^2}=\frac{2n}{h^2}(f_1-f_0). \tag{22}$$

Note that (20) resembles a straightforward discretization of the right side of (2) for large j, since

$$2j\gamma_j = 1 - \gamma_j^2, \quad \gamma_j^2 \le \frac{1}{4j^2+1}. \tag{23}$$

Let us also note that typically f is smooth and even on $r \in (-a, a)$, and hence $f'(0) = 0$, so

$$\lim_{r\to 0} \frac{f'(r)}{r} = f''(0), \quad \text{hence} \quad \lim_{r\to 0} f''(r) + \frac{n-1}{r} f'(r) = nf''(0), \tag{24}$$

which can be compared to (22). In light of these results, we might ponder to what extent (20)–(22) provide a "regularized" discretization of (2).