

Numerical Methods for PDEs

Homework 1

Francisco Jose Castillo Carrasco

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Problem 1

Suppose a double precision floating point number is stored on a computer using 64 bits in the following way: sign 1 bit, exponent 8 bits, and mantissa 55 bits. A given real number r is written as

$$r = \pm m 2^n$$

where the mantissa m satisfies $1/2 \leq m < 1$ and $-128 \leq n \leq 127$. Give the following numbers in both base 2 and base 10 scientific notation:

- (a) What is the largest positive number $realmax$ that can be stored?
- (b) What is the smallest positive number $realmin$ that can be stored?
- (c) What is the machine epsilon ϵ_M (take the leading 1 in m to be a phantom)?

Solution: We calculate the largest positive number as

$$realmax \approx 2^{127} \approx 1.7014 \cdot 10^{38},$$

and the smallest positive number as

$$realmin = 2^{-128} \approx 1.4694 \cdot 10^{-39}.$$

Lastly, the machine epsilon is

$$\epsilon_M = \frac{1}{2} 2^{-55} = 2^{-56} \approx 1.3878 \cdot 10^{-17}$$

Problem 2

- (a) Verify that the three-point central difference formulas for df/dx and d^2f/dx^2 are second-order accurate.

Solution:

We start with the three-point stencil central difference formula for df/dx ,

$$\begin{aligned} \left(\frac{df}{dx}\right)_i &\approx \frac{f_{i+1} - f_{i-1}}{2h} \\ &= \frac{\left(f_i + hf'_1 + \frac{h^2}{2}f''_i + \frac{h^3}{6}f'''_i + \dots\right) - \left(f_i - hf'_1 + \frac{h^2}{2}f''_i - \frac{h^3}{6}f'''_i + \dots\right)}{2h} \\ &= f'_i - \frac{h^2}{6}f'''_i + \dots \\ &= f'_i + \mathcal{O}(h^2), \end{aligned}$$

where $h = \Delta x$. Hence, this approximation for the first derivative is second-order accurate. We continue with the approximation for d^2f/dx^2 ,

$$\begin{aligned} \left(\frac{d^2f}{dx^2}\right)_i &\approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \\ &= \frac{\left(f_i + hf'_1 + \frac{h^2}{2}f''_i + \frac{h^3}{6}f'''_i + \frac{h^4}{24}f^{IV}_i + \dots\right) - 2f_i + \left(f_i - hf'_1 + \frac{h^2}{2}f''_i - \frac{h^3}{6}f'''_i + \frac{h^4}{24}f^{IV}_i + \dots\right)}{h^2} \\ &= f''_i + \frac{h^2}{12}f^{IV}_i + \dots \\ &= f''_i + \mathcal{O}(h^2). \end{aligned}$$

Thus, this approximation is second-order accurate.

- (b) Verify that the one-sided difference formula

$$\frac{du}{dt} \approx \frac{u^{n+1} - u^n}{\Delta t}$$

is first-order accurate.

Solution: Similarly as before,

$$\begin{aligned} \left(\frac{du}{dt}\right)^n &\approx \frac{u^{n+1} - u^n}{\Delta t} \\ &= \frac{\left(u^n + \Delta t \dot{u}^n + \frac{(\Delta t)^2}{2} \ddot{u}^n + \dots\right) - u^n}{\Delta t} \\ &= \dot{u}^n + \frac{\Delta t}{2} \ddot{u}^n + \dots \\ &= \dot{u}^n + \mathcal{O}(\Delta t). \end{aligned}$$

Hence, the one-sided difference formula is first-order accurate.

Problem 3

Verify that the approximation

$$\left(\frac{df}{dx}\right)_i = \frac{1}{\Delta x} \left[-\frac{1}{12}f_{i+2} + \frac{2}{3}f_{i+1} - \frac{2}{3}f_{i-1} + \frac{1}{12}f_{i-2} \right]$$

is fourth-order accurate.

Solution: We start by grouping the previous approximation,

$$\left(\frac{df}{dx}\right)_i = \frac{1}{3h} \left[\frac{1}{4}(f_{i-2} - f_{i+2}) + 2(f_{i+1} - f_{i-1}) \right],$$

and Taylor expanding the terms

$$f_{i\pm 1} = f_i \pm hf'_i + \frac{h^2}{2}f''_i \pm \frac{h^3}{6}f'''_i + \frac{h^4}{24}f^{IV}_i \pm \frac{h^5}{120}f^V_i + \dots,$$

$$f_{i\pm 2} = f_i \pm 2hf'_i + \frac{4h^2}{2}f''_i \pm \frac{8h^3}{6}f'''_i + \frac{16h^4}{24}f^{IV}_i \pm \frac{32h^5}{120}f^V_i + \dots$$

Further, it is easy to check that

$$\begin{aligned} f_{i-2} - f_{i+2} &= -4hf'_i - \frac{16h^3}{6}f'''_i - \frac{64h^5}{120}f^V_i + \dots \\ &= -4hf'_i - \frac{8h^3}{3}f'''_i - \frac{8h^5}{15}f^V_i + \dots, \end{aligned}$$

and

$$\begin{aligned} f_{i+1} - f_{i-1} &= 2hf'_i + \frac{2h^3}{6}f'''_i + \frac{2h^5}{120}f^V_i + \dots \\ &= 2hf'_i + \frac{h^3}{3}f'''_i + \frac{h^5}{60}f^V_i + \dots \end{aligned}$$

Finally, we just substitute in the approximation and obtain

$$\begin{aligned} \left(\frac{df}{dx}\right)_i &= \frac{1}{3h} \left[-hf'_i - \frac{2h^3}{3}f'''_i - \frac{2h^5}{15}f^V_i + 4hf'_i + \frac{2h^3}{3}f'''_i + \frac{2h^5}{60}f^V_i \right] \\ &= \frac{1}{3h} \left[3hf'_i - \frac{3h^5}{30}f^V_i \right] \\ &= f'_i - \frac{h^4}{30}f^V_i \\ &= f'_i + \mathcal{O}(h^4). \end{aligned}$$

Hence, the approximation is indeed fourth order accurate.

Problem 4

Show that the general solution to the heat equation

$$u(x, t) = \int_{-\infty}^{\infty} K(x - y, t) u_0(y) dy$$

where the fundamental solution or kernel

$$K(x, t) = \frac{1}{\sqrt{4\pi\kappa t}} \exp \left\{ -\frac{x^2}{4\kappa t} \right\}$$

does in fact satisfy $u_t = \kappa u_{xx}$ with $u(x, t = 0) = u_0(x)$. *Hint:* First show that K satisfies the heat equation. Then argue that u satisfies the heat equation. Finally show that u satisfies the initial conditions $u(x, t = 0) = u_0(x)$.

Solution: First we calculate the time derivative of K ,

$$K_t(x, t) = \frac{x^2}{4\kappa\sqrt{4\kappa\pi}} \frac{e^{-\frac{x^2}{4\kappa t}}}{t^{5/2}} - \frac{1}{2\sqrt{4\kappa\pi}} \frac{e^{-\frac{x^2}{4\kappa t}}}{t^{3/2}}.$$

Further we calculate the spatial derivatives,

$$K_x(x, t) = -\frac{2x}{4\kappa t\sqrt{4\kappa\pi}} e^{-\frac{x^2}{4\kappa t}},$$

and

$$K_{xx}(x, t) = \frac{x^2}{4\kappa^2\sqrt{4\kappa\pi}} \frac{e^{-\frac{x^2}{4\kappa t}}}{t^{5/2}} - \frac{1}{2\kappa\sqrt{4\kappa\pi}} \frac{e^{-\frac{x^2}{4\kappa t}}}{t^{3/2}}.$$

Finally, it is easy to check that

$$\kappa K_{xx} = \frac{x^2}{4\kappa\sqrt{4\kappa\pi}} \frac{e^{-\frac{x^2}{4\kappa t}}}{t^{5/2}} - \frac{1}{2\sqrt{4\kappa\pi}} \frac{e^{-\frac{x^2}{4\kappa t}}}{t^{3/2}} = K_t(x, t),$$

and that K satisfies the heat equation. Now it is easier to check that u satisfies it as well,

$$\begin{aligned} \kappa u_{xx} &= \kappa \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} K(x - y, t) u_0(y) dy \\ &= \int_{-\infty}^{\infty} \kappa K_{xx}(x - y, t) u_0(y) dy \\ &= \int_{-\infty}^{\infty} K_t(x - y, t) u_0(y) dy \\ &= \frac{\partial}{\partial t} \int_{-\infty}^{\infty} K(x - y, t) u_0(y) dy \\ &= \frac{\partial}{\partial t} u(x, t) \\ &= u_t. \end{aligned}$$

To check that the initial condition is satisfied by this solution we take the limit,

$$\begin{aligned}
\lim_{t \rightarrow 0} u(x, t) &= \lim_{t \rightarrow 0} \int_{-\infty}^{\infty} K(x - y, t) u_0(y) dy \\
&= \int_{-\infty}^{\infty} \lim_{t \rightarrow 0} K(x - y, t) u_0(y) dy \\
&= \int_{-\infty}^{\infty} \delta(x - y) u_0(y) dy \\
&= u_0(x),
\end{aligned}$$

where we have used the fact that the limit at time zero of the heat kernel is the Dirac delta and its properties.

Problem 5

Show that the TR method for the heat equation $u_t = u_{xx}$

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{2\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n + u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1})$$

is second-order accurate, using the definition of the local truncation.

Solution:

Let $\Delta x = h$. We then substitute the true solution into the TR method and Taylor expand to find,

$$\begin{aligned}
u(x, t + \Delta t) &= u(x, t) + \frac{\Delta t}{2} \left(u_{xx}(x, t) + \frac{h^2}{12} u_{xxxx}(x, t) + \cdots \right) \\
&\quad + \frac{\Delta t}{2} \left(u_{xx}(x, t + \Delta t) + \frac{h^2}{12} u_{xxxx}(x, t + \Delta t) + \cdots \right) + \Delta t \tau.
\end{aligned}$$

Letting $u(x, t) = u$ and Taylor expanding again, we find,

$$\begin{aligned}
u + \Delta t u_t + \frac{\Delta t^2}{2} u_{tt} + \cdots &= u + \frac{\Delta t}{2} \left(u_{xx}(x, t) + \frac{h^2}{12} u_{xxxx}(x, t) + \cdots \right) \\
&\quad + \frac{\Delta t}{2} \left(u_{xx} + \Delta t u_{xxt} + \frac{\Delta t^2}{2} u_{xxtt} + \cdots \right) \\
&\quad + \frac{\Delta t h^2}{24} \left(u_{xxxx} + \Delta t u_{xxxxt} + \frac{\Delta t^2}{2} u_{xxxxtt} + \cdots \right) \\
&\quad + \Delta t \tau.
\end{aligned}$$

Making use of the differential equation $u_t = u_{xx}$,

$$\begin{aligned}
u + \Delta t u_t + \frac{\Delta t^2}{2} u_{tt} + \cdots &= u + \Delta t u_t + \frac{\Delta t^2}{2} u_{tt} \\
&\quad + \frac{\Delta t h^2}{12} u_{xxxx} + \frac{\Delta t^3}{4} u_{xxtt} + \frac{\Delta t^2 h^2}{24} u_{xxxxt} + \frac{\Delta t^3 h^2}{48} u_{xxxxtt} \\
&\quad + \Delta t \tau + \dots
\end{aligned}$$

Solving for τ , and noting the fact that $u_t = u_{xx}$, we get

$$\tau = \frac{-u_{xxtt}}{4}\Delta t^2 + \frac{-u_{xxxx}}{12}h^2 + \dots .$$

Hence, the TR method for the heat equation is second-order accurate.