MATH521
Numerical Analysis of Partial Differential Equations

Winter 2017/18, Term 2
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Homework Assignment 4

Please submit the following files as indicated below: source code PDF file image file video file

Question 1 | **4 marks** | Today we will solve the steady advection-diffusion equation in 1D

$$\begin{aligned} au' - Du'' &= 0 \qquad \text{in }]0,1[\\ u(0) &= 0 \\ u(1) &= 1 \end{aligned}$$

where, for simplicity, we assume the advection velocity $a \geq 0$ and the diffusivity $D > 0$ to be constant throughout the domain.

(a) Discretise the advection-diffusion problem using the $N+1$ grid points

$$x = 0, h, 2h, 3h, \ldots, (N-1)h, 1,$$

(where $h = 1/N$) with the second-order consistent central difference approximation

$$u'(x) \approx \frac{u(x+h) - u(x-h)}{2h}.$$

Write down the 'big linear system' $L^h_{\text{CD}} u^h = f^h$ (the first two rows and the last row suffice).

For what range of h-values does the matrix L^h_{CD} satisfy the M-matrix criterion 'weakly chained diagonally dominant & L-matrix'?

Hint: The identity

$$|\alpha + \beta| + |\alpha - \beta| = 2 \max \{\, |\alpha|, |\beta| \,\}$$

may be useful.

With the above central difference approximation, the 'big linear system' reads

$$\left[\frac{a}{2h} \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & & \ddots & & \\ & & & -1 & 0 \end{pmatrix} + \frac{D}{h^2} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & & -1 & 2 \end{pmatrix} \right] \begin{pmatrix} u^h_1 \\ u^h_2 \\ \vdots \\ u^h_{N-1} \end{pmatrix} = \begin{pmatrix} f(h) \\ f(2h) \\ \vdots \\ f((N-1)h) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ -\frac{a}{2h} + \frac{D}{h^2} \end{pmatrix}.$$

For the matrix of this system to satisfy the M-criterion, we need the following:

- L^h_{CD} must be weakly diagonally dominant in all rows.

  This is true if and only if

$$\begin{aligned} \frac{2D}{h^2} &\geq \left| \frac{a}{2h} - \frac{D}{h^2} \right| && \text{(from Eq 1)} \\ \frac{2D}{h^2} &\geq \left| -\frac{a}{2h} - \frac{D}{h^2} \right| + \left| \frac{a}{2h} - \frac{D}{h^2} \right| = \left| \frac{a}{2h} + \frac{D}{h^2} \right| + \left| \frac{a}{2h} - \frac{D}{h^2} \right| = 2\max\left\{ \frac{a}{2h}, \frac{D}{h^2} \right\} && \text{(from Eq 2 to } N-2\text{)} \\ \frac{2D}{h^2} &\geq \left| -\frac{a}{2h} - \frac{D}{h^2} \right| = \frac{a}{2h} + \frac{D}{h^2} && \text{(from Eq } N-1\text{)} \end{aligned}$$

According to the second inequality, we need

$$\frac{a}{2h} \leq \frac{D}{h^2} \qquad \Leftrightarrow \qquad h \leq \frac{2D}{a}$$

and in this case the first and last inequalities are already met as well.

- L^h_{CD} must be strictly diagonally dominant in at least one row.

  Consider again the first equation of the 'big linear system' under the constraint

  $$h \leq \frac{2D}{a}.$$

  The absolute value of the off-diagonal term is

  $$\left|\frac{a}{2h} - \frac{D}{h^2}\right| = \frac{D}{h^2} - \frac{a}{2h} \leq \frac{D}{h^2} < \frac{2D}{h^2},$$

  so L^h_{CD} is strictly diagonally dominant in the first row.

- L^h_{CD} must possess the weak chain property.

  Note that this matrix is of the form

  $$\begin{pmatrix} \star & ? & & & \\ \star & \star & ? & & \\ & & \ddots & & \\ & & \star & \star \end{pmatrix}$$

  where the entries marked with an asterisk are guaranteed to be non-zero while the upper diagonal terms marked with a question mark might cancel. Hence, starting in any row i_0, the chain $i_0 \to i_0 - 1 \to i_0 - 2 \to \cdots \to 1$ is admissible in the sense that the matrix entry corresponding to each step is non-zero.

- L^h_{CD} must be an L-matrix.

  All diagonal entries are generally positive and under the above restriction $h \leq \frac{2D}{a}$, then all off-diagonal entries are non-positive.

Overall: the matrix L^h_{CD} is an M-matrix provided that the mesh is sufficiently fine, $h \leq \frac{2D}{a}$.

(b) Leaving everything else unchanged, discretise the transport term with the first-order consistent upwind[1] differencing scheme

$$u'(x) \approx \frac{u(x) - u(x-h)}{h}$$

instead. Write down the 'big linear system' $L^h_{\mathrm{UD}} u^h = f^h$.

For what range of h-values does the matrix L^h_{UD} satisfy the M-matrix criterion?

Mutatis mutandis, we get

$$\left[\frac{a}{h} \begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & & \ddots & \\ & & -1 & 1 \end{pmatrix} + \frac{D}{h^2} \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & \\ & & -1 & 2 \end{pmatrix} \right] \begin{pmatrix} u^h_1 \\ u^h_2 \\ \vdots \\ u^h_{N-1} \end{pmatrix} = \begin{pmatrix} f(h) \\ f(2h) \\ \vdots \\ f((N-1)h) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \frac{D}{h^2} \end{pmatrix}.$$

For the matrix of this system to satisfy the M-criterion, we need the following:

- L^h_{UD} must be weakly diagonally dominant in all rows.

  This is true if and only if

  $$\begin{aligned} \frac{a}{h} + \frac{2D}{h^2} &\geq \left| -\frac{D}{h^2} \right| = \frac{D}{h^2} && \text{(from Eq 1)} \\ \frac{a}{h} + \frac{2D}{h^2} &\geq \left| -\frac{a}{h} - \frac{D}{h^2} \right| + \left| -\frac{D}{h^2} \right| = \frac{a}{h} + \frac{D}{h^2} + \frac{D}{h^2} && \text{(from Eq 2 to } N-2) \\ \frac{a}{h} + \frac{2D}{h^2} &\geq \left| -\frac{a}{h} - \frac{D}{h^2} \right| = \frac{a}{h} + \frac{D}{h^2} && \text{(from Eq } N-1) \end{aligned}$$

  These inequalities hold for all $h > 0$

- L^h_{UD} must be strictly diagonally dominant in at least one row.

  Clearly, the matrix is strictly diagonally dominant in the first and the last row.

- L^h_{UD} must possess the weak chain property.

  This matrix is of the form

  $$\begin{pmatrix} \star & \star & & \\ \star & \star & \star & \\ & & \ddots & \\ & & \star & \star \end{pmatrix}$$

  where the entries marked with an asterisk are guaranteed to be non-zero. This includes in particular the $\star$-entries of the matrix L^h_{CD} in part (a) and hence the chain property still holds.

- L^h_{UD} must be an L-matrix.

  All diagonal entries are generally positive and all off-diagonal entries are generally non-positive.

[1]Upwind differencing uses a one-sided difference quotient. The two-point stencil covers the point x itself and the nearest point in 'upwind' direction, where the flow is coming from.

(c) Download the file `advection_diffusion.m` and read the output of `help advection_diffusion`. Everything else is intentionally obfuscated so that you still have to do (a) and (b) yourself! You can however use this function to check your answers for the admissible ranges of h in (a) and (b).

What do you observe if the matrix L^h is not an M-matrix? Use your knowledge from lectures and the technical language you have learnt so far to *describe* and *explain* your observations.

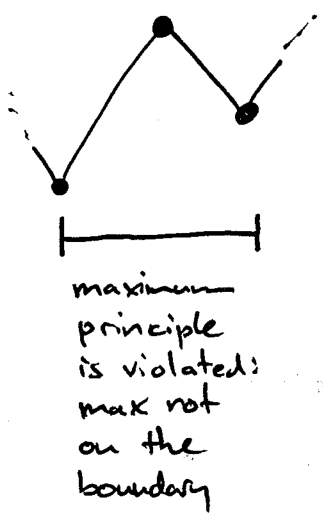
When the matrix L^h is not an M-matrix, then the numerical solution of this advection-diffusion problem may exhibit strongly oscillatory behaviour with large overshoots and undershoots compared to the exact solution.

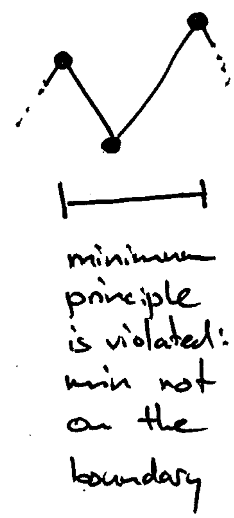
The exact solution satisfies a maximum and a minimum principle: $0 \leq u(x) \leq 1$ for all $x \in [0, 1]$. When L^h is not an M-matrix, we have no guarantee that $u^h \geq 0$ provided that $L^h u^h \geq 0$ (and due to the potentially negative boundary term $-\frac{a}{2h} + \frac{D}{h^2}$ on the right hand side of the central differencing scheme, $L^h u^h$ may not even be nonnegative). Indeed, the numerical solution may become negative when the M-criterion is violated.

The exact solution cannot even possess any (strict) local maxima or minima in the interior of the domain: assume that u has a strict local maximum/minimum at $x^* \in]0, 1[$ and apply the maximum/minimum principle on a small interval $]x^* - \epsilon, x^* + \epsilon[$ around this point to obtain that

$$\min \{ u(x^* - \epsilon), u(x^* + \epsilon) \} \leq u(x^*) \leq \max \{ u(x^* - \epsilon), u(x^* + \epsilon) \}$$

but this contradicts the assumption of a strict local maximum/minimum at x^*. However, without the M-matrix property, the numerical solution may well exhibit spurious local maxima and minima.





Note that both the central and the upwind difference approximations are consistent, stable and convergent: for sufficiently small h, there are no issues with the central difference scheme at all. However, for strongly advection-dominated problems with h not insanely tiny, **the numerical solutions are complete nonsense because they violate the maximum principle**, a characteristic feature of the exact solution. I hope that I have now convinced you that maximum principles and M-matrices are really important, for mathematicians, scientists and engineers alike!

(d) Even though the upwind differencing scheme is only first-order consistent as an approximation of the equation

$$au' - Du'' = 0$$

it is second-order consistent as an approximation of a slightly different equation,

$$au' - (D + \tilde{D})u'' = 0,$$

provided that $u \in C^4([0,1])$. Calculate this number $\tilde{D}$.

Hint: Use TAYLOR expansions as done in class or video #7 to determine the truncation error

$$au'(x) \quad - \quad \text{(upwind difference approximation of this term)}\,.$$

$\tilde{D}$ will depend on h.

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(\xi)$$

for some $\xi \in]x-h, x[$. Hence,

$$au'(x) - a\frac{u(x) - u(x-h)}{h} = a\frac{h}{2}u''(x) - a\frac{h^2}{6}u'''(\xi).$$

Combining this with the discrete diffusion term, we obtain

$$au'(x) - Du''(x) - a\frac{h}{2}u''(x) = -a\frac{u(x) - u(x-h)}{h} + D\frac{-u(x+h) + 2u(x) - u(x-h)}{h} + O(h^2)$$

provided that $u \in C^4([0,1])$.

This extra diffusivity $\tilde{D} = \frac{ah}{2}$ is called *numerical diffusion*.

In conclusion, the central difference approximation of the advection term may produce nonsense, but the upwind difference approximation is usually very inaccurate as an approximation of the original equation since $\tilde{D}$ can be quite large for advection-dominated problems and it only decreases very slowly as the grid is refined. $\tilde{D}$ has the effect that steep gradients are smeared out. As can be seen from the program in (c), the upwind difference solution has a much more gentle incline near the right endpoint than the exact solution.

Overall, neither the central differencing scheme nor the upwind differencing scheme is generally well-suited for advection-diffusion problems: central differencing may give rise to spurious extrema while upwind differencing is too inaccurate. Towards the end of this course we'll learn how to fix this: we'll start from the inaccurate but otherwise sensible upwind-difference solution, but then we'll subtract all of $\tilde{D}$ in regions where numerical diffusion is not needed and as much of $\tilde{D}$ as possible otherwise. This will give us a numerical solution which is 2$^{\text{nd}}$ order accurate in regions where the solution is smooth and where it satisfies the maximum/minimum principle anyways, and between 1$^{\text{st}}$ and 2$^{\text{nd}}$ order accurate where numerical diffusion is needed to avoid violations of the maxmimum/minimum principle.

Your Primer Talk | **1 mark** | Open the primer talk assignment on Canvas, where you can find a worksheet that will help you prepare an effective primer talk. You will give your 2-3 minute talk on Thursday, 8 February during regular lecture times. You don't have to use any visual aids for this very short talk, but you may if you wish.

Please give me the following information on your talk when you submit this assignment and I will give you 1 mark for that:

- Are you going to use the document camera (which I use to project my paper notes to the screen)?

  ◯ Yes / Probably ◯ No

  If you're planning to connect your own device to the projector, please tick 'No'.

- Purpose of your talk (from the talk preparation worksheet): By the end of this talk, the audience should be able to...

Your Learning Progress | What is the one most important thing that you have learnt from this assignment?

What is the most substantial new insight that you have gained from this course this week? Any *aha moment*?