Columbia Engineering
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APMAE4302

Methods in computational science

Homework 2

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1 Problem 1

1) First, let's assume that there are two problems described by:

$$\mathbf{Au} = \mathbf{b} \qquad \text{and} \qquad \mathbf{A\hat{u}} = \mathbf{\hat{b}} \tag{1}$$

By subtracting both:

$$\mathbf{Au} - \mathbf{A\hat{u}} = \mathbf{b} - \mathbf{\hat{b}} \tag{2}$$
$$\mathbf{A}(\mathbf{u} - \mathbf{\hat{u}}) = \mathbf{b} - \mathbf{\hat{b}} \tag{3}$$
$$\rightarrow (\mathbf{u} - \mathbf{\hat{u}}) = \mathbf{A}^{-1}(\mathbf{b} - \mathbf{\hat{b}}) \tag{4}$$

Considering $||\mathbf{Ax}|| \leq ||\mathbf{A}||||\mathbf{x}||$

$$||\mathbf{A}(\mathbf{u} - \mathbf{\hat{u}})|| \leq \|\mathbf{A}\|\|(\mathbf{u} - \mathbf{\hat{u}})\| = \|\mathbf{A}\|\|\mathbf{A}^{-1}(\mathbf{b} - \mathbf{\hat{b}})\| \leq \|\mathbf{A}\|\|\mathbf{A}^{-1}\|\|(\mathbf{b} - \mathbf{\hat{b}})\| \tag{5}$$

Thus:

$$\|\mathbf{A}\|\|(\mathbf{u} - \mathbf{\hat{u}})\| \leq \|\mathbf{A}\|\|\mathbf{A}^{-1}\|\|(\mathbf{b} - \mathbf{\hat{b}})\| = \kappa(\mathbf{A})\|(\mathbf{b} - \mathbf{\hat{b}})\| \tag{6}$$

Also, it can be established that$\|\mathbf{Au}\| = \|\mathbf{b}\| \leq \|\mathbf{A}\|\|\mathbf{u}\|$, and therefore $\frac{\|\mathbf{b}\|}{\|\mathbf{u}\|} \leq \|\mathbf{A}\|$

By multiplying both sides by $\|(\mathbf{u} - \mathbf{\hat{u}})\|$

$$\frac{\|\mathbf{b}\|}{\|\mathbf{u}\|}\|(\mathbf{u} - \mathbf{\hat{u}})\| \leq \|\mathbf{A}\|\|(\mathbf{u} - \mathbf{\hat{u}})\| \tag{7}$$

Therefore, using Equations (6) and (7):

$$\frac{\|\mathbf{b}\|}{\|\mathbf{u}\|}\|(\mathbf{u} - \mathbf{\hat{u}})\| \leq \kappa(\mathbf{A})\|(\mathbf{b} - \mathbf{\hat{b}})\| \tag{8}$$
$$\rightarrow \frac{\|\mathbf{u} - \mathbf{\hat{u}}\|}{\|\mathbf{u}\|} \leq \kappa(\mathbf{A})\frac{\|(\mathbf{b} - \mathbf{\hat{b}})\|}{\|\mathbf{b}\|} \tag{9}$$

2)

From equation 3:

$$||\mathbf{A}(\mathbf{u}-\hat{\mathbf{u}})|| \leq \|\mathbf{A}\|\|(\mathbf{u}-\hat{\mathbf{u}})\| \rightarrow ||\mathbf{r}|| \leq \|\mathbf{A}\|\|\mathbf{e}\| \tag{10}$$

Also, as $\mathbf{u} = \mathbf{A}^{-1}\mathbf{b}$, then:

$$\|\mathbf{u}\| = \|\mathbf{A}^{-1}\mathbf{b}\| \leq \|\mathbf{A}^{-1}\|\|\mathbf{b}\| \tag{11}$$

Multiplying Equation (10) by Equation (11):

$$\begin{align} ||\mathbf{r}||\|\mathbf{u}\| &\leq \|\mathbf{A}^{-1}\|\|\mathbf{A}\|\|\mathbf{b}\|\|\mathbf{e}\| \tag{12} \\ ||\mathbf{r}||\|\mathbf{u}\| &\leq \kappa(\mathbf{A})\|\mathbf{b}\|\|\mathbf{e}\| \tag{13} \\ \frac{1}{\kappa(\mathbf{A})}\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} &\leq \frac{\|\mathbf{e}\|}{\|\mathbf{u}\|} \tag{14} \end{align}$$

Since $\|\mathbf{e}\| = \|\mathbf{u}-\hat{\mathbf{u}}\|$ it follows that:

$$\frac{1}{\kappa(\mathbf{A})}\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} \leq \frac{\|\mathbf{e}\|}{\|\mathbf{u}\|} \leq \kappa(\mathbf{A})\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} \tag{15}$$

2 Problem 2

If $\mathbf{v}_j = \sin(j\pi x_i)$ is an eigenvector of $\mathbf{A}$, then it satisfies $\mathbf{A}\mathbf{v}_j = \lambda_j \mathbf{v}_j$.

$$\begin{align} (\mathbf{A}\mathbf{v}_j)_i &= \frac{1}{h^2}(-v^{i-1} + 2v^i - v^{i+1}) \tag{16} \\ &= \frac{1}{h^2}(-\sin(j\pi(i-1)h) + 2\sin(j\pi(i)h) - \sin(j\pi(i+1)h) \tag{17} \end{align}$$

Define the angles $\theta = j\pi ih$ and $\phi = j\pi h$.

$$\begin{aligned} (\mathbf{A}\mathbf{v}_j)_i &= \frac{1}{h^2}(-\sin(\theta-\phi) + 2\sin(\theta) - \sin(\theta+\phi)) \\ &= \frac{1}{h^2}(-\sin(\theta)\cos(\phi) + \sin(\phi)\cos(\theta) + 2\sin(\theta) - \sin(\theta)\cos(\phi) - \sin(\phi)\cos(\theta)) \\ &= \frac{1}{h^2}(-2\sin(\theta)\cos(\phi) + 2\sin(\theta)) \\ &= \frac{1}{h^2}(2\sin(\theta)(1-\cos(\phi))) \end{aligned}$$

And $1 - \cos(\phi) = 2\sin^2(\frac{\phi}{2})$

$$
\begin{aligned}
(\mathbf{A}\mathbf{v}_j)_i &= \frac{4}{h^2}(\sin^2(\frac{\phi}{2}))\sin(\theta) = \frac{4}{h^2}(\sin^2(\frac{j\pi h}{2}))\sin(j\pi i h) = \frac{4}{h^2}(\sin^2(\frac{j\pi h}{2}))\sin(j\pi x_i) \\
&= \frac{4}{h^2}(\sin^2(\frac{j\pi h}{2}))\mathbf{v_j}
\end{aligned}
$$

This shows that $\mathbf{v}_j$ corresponds to an eigenvector of $\mathbf{A}$.

2) The corresponding eigenvalue λ is the scalar multiplying the eigenvector.

$$(\mathbf{A}\mathbf{v}_j)_i = \frac{4}{h^2}(\sin^2(\frac{j\pi h}{2}))\mathbf{v_j} = \lambda_j \mathbf{v_j}$$

Then:

$$\lambda_j = \frac{4}{h^2}\sin^2(\frac{j\pi h}{2}) = 4m^2\sin^2(\frac{j\pi}{2m}) \tag{18}$$

For $j = 1, \ldots, m-1$ (excluding the boundary nodes, where λ is not defined in the same way).

3) If $m \to \infty$:

- For $j = 1$, we obtain the smallest eigenvalue. Since $\frac{\pi}{2m}$ is small, we use $\sin\left(\frac{\pi}{2m}\right) \approx \frac{\pi}{2m}$. Then:

$$\lambda_{\min} \approx 4m^2\left(\frac{\pi}{2m}\right)^2 = \pi^2 \tag{19}$$

- For $j = m-1$, we obtain the largest eigenvalue. Since

$$\frac{(m-1)\pi}{2m} = \frac{\pi}{2} - \frac{\pi}{2m} \approx \frac{\pi}{2},$$

we have $\sin\left(\frac{\pi}{2}\right) = 1$. Then:

$$\lambda_{\max} \approx 4m^2 \tag{20}$$

Finally:

$$\kappa(\mathbf{A}) \approx \frac{4m}{\pi} = O(m^2) \tag{21}$$

3 Problem 3

a)

$$u(x) = \sin(k\pi x) + c(x - \frac{1}{2})^3 \tag{22}$$
$$u'(x) = k\pi \cos(k\pi x) + 3c(x - \frac{1}{2})^2 \tag{23}$$
$$u''(x) = -k^2\pi^2 \sin(k\pi x) + 6c(x - \frac{1}{2}) \tag{24}$$

Then, by susbtituting in $-u'' + \gamma u = f(x)$

$$k^2\pi^2 \sin(k\pi x) - 6c(x - \frac{1}{2}) + \gamma(\sin(k\pi x) + c(x - \frac{1}{2})^3) = f(x) \tag{25}$$
$$(k^2\pi^2 + \gamma) \sin(k\pi x) + \gamma c(x - \frac{1}{2})^3 - 6c(x - \frac{1}{2}) = f(x) \tag{26}$$

b)

For this problem, the code was implemented in a file named bvp.c, located in the main HW2 directory. The file was developed based on the tri.c code and modified by adding the term γu. As a result, the matrix $\mathbf{A}$ takes the following form:

$$\mathbf{A}_i = \frac{1}{h^2} \begin{bmatrix} -1 & 2 + \gamma & -1 \end{bmatrix}] \tag{27}$$

The right-hand side vector is given by $\mathbf{b} = f(x_i)$.

Using the provided plotting code and running the bvp.c program, the following plot is obtained:

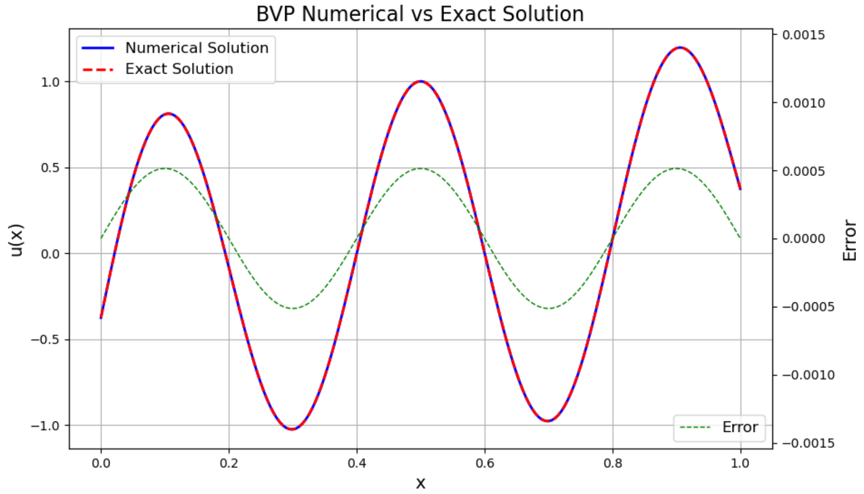

Figure 1: Numerical vs exact solution

c) By setting $\gamma = 0$ and $c = 0$, and using 1 MPI process, the following convergence plot is obtained:

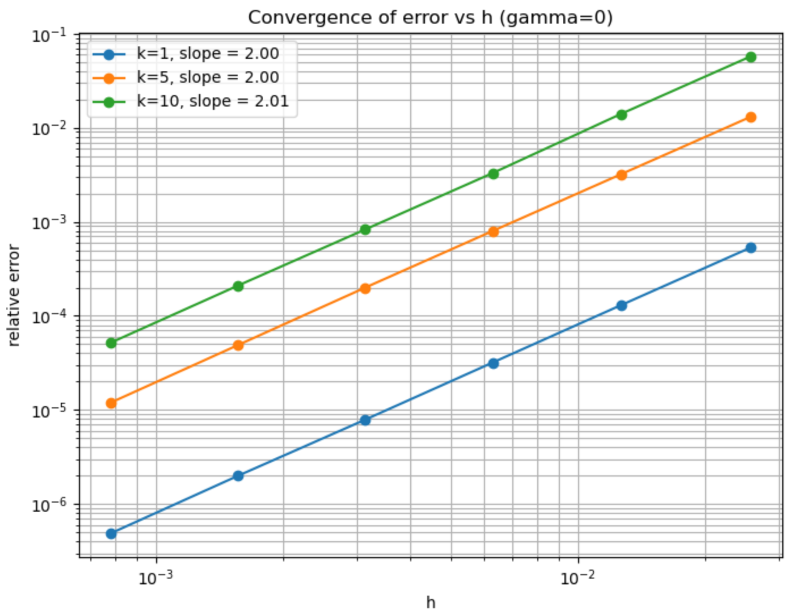

Figure 2: Convergence plot

It can be observed that the order of convergence is 2 for all values of k.

4 Problem 4

(a) Jacobi preconditioned Richardson (**10000 iterations**): Very slow convergence. The method essentially stagnates, since Richardson is highly sensitive to the condition number and Jacobi preconditioning is not sufficient to significantly improve convergence.

(b) Unpreconditioned Conjugate Gradient (**102 iterations**): Significant improvement over Richardson. However, it still requires many iterations due to the condition number of the system and the absence of preconditioning.

(c) Unpreconditioned Conjugate Gradient with $c = 0$ (**1 iteration**): Converges in a single iteration. This occurs because the right hand side aligns with an eigenvector of the matrix, allowing to recover the exact solution immediately.

(d) ICC preconditioned Conjugate Gradient (**1 iteration**): Excellent performance. The ICC preconditioner provides a very accurate approximation of the matrix factorization, resulting in a well conditioned system.

(e) Block Jacobi preconditioned CG (4 processors, **7 iterations**): Slower than ICC. The preconditioning is applied locally to each block rather than globally, which reduces its effectiveness due to loss of global coupling.

(f) MUMPS direct solver (1 processor, **1 iteration**): Direct solver, so the solution is obtained exactly in one step. No iterative process is required.

(g) MUMPS direct solver (4 processors, **1 iteration**): Same behavior as with one processor. Parallelization improves computational time, but not the number of iterations.