MATHEMATICS 714 HOMEWORK 2

A PREPRINT

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A

(a) If we have $v \in \text{span}\{w_1, w_2, \dots, w_n\}$ then $v = a_1 w_1 + a_2 w + 2 + \cdots + a_n w_n$ for some set of scalars a_i. We can then take the inner product of both sides with w_k for $k = 1, 2, ..., n$ to find

$$\begin{aligned}\langle v, w_k \rangle &= \langle a_1 w_1 + a_2 w + 2 + \cdots + a_n w_n, w_k \rangle \\ &= \sum_{i=1}^{n} a_i \langle w_i, w_k \rangle \\ &= a_k \|w_k\|.\end{aligned}$$

Therefore $a_k = \frac{\langle v, w_k \rangle}{\|w_k\|^2}$ so

$$v = \sum_{j=1}^{n} \frac{\langle v, w_j \rangle}{\|w_j\|^2} w_j.$$

(b) (i) The number of iterations to convergence may be strictly smaller than N because if we have an initial guess such that the solution lies in a Krylov subspace we can converge sooner than N iterations.

(ii) Our base case is $n = 1$ so the only allowable j value is $j = 0$. We have $p_0 = r_0$ and $r_0 = f - Ax_0$. We also have $p_1 = r_1 - \frac{\langle r_1, p_0 \rangle_A}{\|p_0\|_A^2} r_0 = r_1 - \frac{\langle r_1, r_0 \rangle_A}{\|r_0\|_A^2} r_0$. The algorithm gives $w_0 = Ar_0$ and $\alpha_0 = \frac{\|r_0\|^2}{p_0^T w_0} = \frac{\|r_0\|^2}{\|r_0\|_A^2}$. Therefore $r_1 = r_0 - \alpha_0 w_0 = r_0 - \frac{\|r_0\|^2}{\|r_0\|_A^2} Ar_0$. Now we show

$$\begin{aligned}\langle p_1, p_0 \rangle_A &= \langle p_1, r_0 \rangle_A \\ &= r_1^T A r_0 - \frac{\langle r_1, r_0 \rangle_A}{\|r_0\|_A^2} \langle r_0, r_0 \rangle_A \\ &= \langle r_1, r_0 \rangle_A - \frac{\|r_0\|_A^2}{\|r_0\|_A^2} \langle r_1, r_0 \rangle_A \\ &= 0.\end{aligned}$$

Now for the induction step assume that for $k < n$, with $0 \le l < k < n \le n^* - 1$ we have $\langle p_k, p_j \rangle_A = 0$. We want to show that for $0 \le l < n \le n^* - 1$ we still have $\langle p_n, p_l \rangle_A = 0$. Note that by our induction hypothesis, $\langle p_j, p_l \rangle = 0$ when $j \ne l$ and $\max l, j < n$. By our formula for p_n, we get

$$\begin{aligned}\langle p_n, p_l \rangle_A &= \langle r_n, p_l \rangle_A - \sum_{j=0}^{n-1} \frac{\langle r_n, p_j \rangle_A}{\|p_j\|_A^2} \langle p_j, p_l \rangle_A \\ &= \langle r_n, p_l \rangle_A - \frac{\langle p_l, p_l \rangle_A}{\|p_l\|_A^2 \langle r_n, p_l \rangle_A} \\ &= \langle r_n, p_l \rangle - \frac{\|p_l\|_A^2}{\|p_l\|_A^2} \langle r_n, p_l \rangle_A \\ &= 0.\end{aligned}$$

(c) (i) Since $\{\phi_n\}$ form an orthonormal basis for $\mathbb{R}^N$, we have $v, w \in \text{span}\{\phi_1, \ldots, \phi_N\}$ and $\|\phi_n\| = 1$. Thus by part (a), we can write $v = \sum_{n=1}^{N} \langle v, \phi_n \rangle \phi_n$. Therefore

$$\langle Av, w \rangle = \sum_{n=1}^{N} \langle v, \phi_n \rangle \langle A\phi_n, w \rangle = \sum_{n=1}^{N} \langle v, \phi_n \rangle \langle \lambda_n \phi_n, w \rangle = \sum_{n=1}^{N} \lambda_n \langle v, \phi_n \rangle \langle \phi_n, w \rangle.$$

(ii) For $1 \leq n \leq N$, since A is positive definite we have $\phi_n^T A \phi_n > 0$, but $A\phi_n = \lambda_n \phi_n$ so $\phi_n^T A \phi_n = \lambda_n \|\phi_n\|^2 > 0$ which implies $\lambda_n > 0$.

(iii) Note that $\|v\|^2 = \sum_{n=1}^{N} \langle v, \phi_n \rangle^2$ and $Av = \sum_{n=1}^{N} \langle v, \phi_n \rangle A\phi_n = \sum_{n=1}^{N} \langle v, \phi_n \rangle \lambda_n \phi_n$. Then since $\langle \pi_n, \phi_m \rangle = \delta_{n,m}$,

$$\langle Av, v \rangle = \sum_{j=1}^{N} \sum_{n=1}^{N} \langle v, \phi_n \rangle \langle v, \phi_j \rangle \lambda_n \langle \phi_n, \phi_j \rangle = \sum_{n=1}^{N} \langle v, \phi_n \rangle^2 \|\phi_n\|^2 \lambda_n.$$

Therefore $\lambda_1 \|v\|^2 \leq \langle Av, v \rangle \leq \lambda_N \|v\|^2$.

(iv) We can write $\|v\|^2 = \sum_{j=1}^{N} \langle v, \phi_j \rangle^2$. Note that $Av = \sum_{j=1}^{N} \langle v, \phi_j \rangle A\phi_j = \sum_{j=1}^{N} \langle v, \phi_j \rangle \lambda_j \phi_j$, and $A^T = A$ since A is symmetric. Then

$$\begin{aligned}
\|Av\|^2 &= \langle Av, Av \rangle \\
&= v^T A \sum_{j=1}^{N} \langle v, \phi_j \rangle \lambda_j \phi_j \\
&= v^T \sum_{j=1}^{N} \langle v, \phi_j \rangle \lambda_j^2 \phi_j \\
&= \sum_{j=1}^{N} \sum_{k=1}^{N} \langle v, \phi_j \rangle \langle v, \phi_k \rangle \lambda_j^2 \langle \phi_j, \phi_k \rangle \\
&= \sum_{j=1}^{N} \langle v, \phi_j \rangle^2 \lambda_j^2 \\
&\leq \lambda_N^2 \sum_{j=1}^{N} \langle v, \phi_j \rangle^2.
\end{aligned}$$

Therefore $\|Av\| \leq \lambda_N \|v\|$.

(d) By definition, $p_{n+1} = r_{n+1} + \beta_n p_n$. From the algorithm, $w_n = Ap_n$ so $r_{n+1} = r_n - \alpha_n w_n = r_n - \alpha_n A p_n$. From the formula for p we find $p_n = r_n + \beta_{n-1} p_{n-1}$ so we can write $r_n = p_n - \beta_{n-1} p_{n-1}$. Therefore our equation for r_{n+1} becomes $r_{n+1} = p_n - \beta_{n-1} p_{n-1} - \alpha_n A p_n$. Substituting this in to our equation for p_{n+1} gives

$$p_{n+1} = p_n - \beta_{n-1} p_{n-1} - \alpha_n A p_n + \beta_n p_n = (1 + \beta_n) p_n - \alpha_n p_n - \beta_{n-1} p_{n-1}$$

(e) By the Cayley-Hamilton theorem, since A is nonsingular, we have

$$A^n + c_{N-1} A^{N-1} + \cdots + c_1 A + (-1)^N \det(A) I = 0$$

for constants $c_n, \ldots, c_1$ based on the eigenvalues of A. We can then write

$$A^N = -c_{N-1} A^{N-1} - \cdots - c_1 A + (-1)^{N-1} \text{det}(A) I$$

and since $\text{det} A \neq 0$ we have at least one nonzero coefficient, and $A^N \neq 0$, so A^N is a linear combination of $I, A, A^2, \ldots, A^{N-1}$.

(f) (i) By definition,

$$\begin{aligned}
e_{n+1} &= u_{n+1} - u \\
&= u_n + \alpha f - \alpha A u_n - u - \alpha f + \alpha A u \\
&= (u_n - u) - \alpha A (u_n - u) \\
&= (I - \alpha A) e_n.
\end{aligned}$$

(ii) Since $\|I-\alpha A\| \le \rho$, and by (i) we have $e_{n+1}=(I-\alpha A)e_n$, $\|e_{n+1}\| \le \|I-\alpha A\|\|e_n\| \le \rho\|e_n\|$.

(iii) Since λ_1 and λ_N are the largest and smallest eigenvalues,

$$\rho = \max_{i\le j\le N} |1-\alpha\lambda_j| = \max\{|1-\alpha\lambda_1|, |1-\alpha\lambda_N\}.$$

As we make one of those terms smaller we make the other bigger, so the optimal α makes the two equal. This happens when α is the reciprocal of the average, so $\alpha = \frac{2}{\lambda_1+\lambda_N}$.

(iv) Since ρ is determined by λ_1 and λ_N, we first consider

$$\begin{aligned}|1-\alpha\lambda_1| &= \left|1-\frac{2\lambda_1}{c+C}\right| \\ &= \left|\frac{c+C-2\lambda_1}{c+C}\right| \\ &\le \left|\frac{c+C-2c}{c+C}\right| \\ &= \left|\frac{C-c}{C+c}\right|.\end{aligned}$$

Next we consider

$$\begin{aligned}|1-\alpha\lambda_N| &= \left|1-\frac{2\lambda_N}{c+C}\right| \\ &= \left|\frac{c+C-2\lambda_N}{c+C}\right| \\ &\le \left|\frac{C-c}{c+C}\right|.\end{aligned}$$

Therefore $\rho \le |C-c|/|C+c|$.

(g) (i) From the algorithm $p_0 = r_0$ so $w_0 = Ap_0 = Ar_0$. Therefore $r_1 = \alpha_0 w_0 = r_0 - \alpha_0 Ar_0$.

(ii) We begin with the formula for r_n, substituting $w_{n-1} = Ap_{n-1}$, to find $r_n = r_{n-1} - \alpha_{n-1}Ap_{n-1}$ which gives $Ap_{n-1} = \frac{1}{\alpha_{n-1}}(r_{n-1}-r_n)$. Then, from the update formula for p_n, using the identity we just found for Ap_{n-1}, we find

$$w_n = Ap_n = Ar_n + \beta_{n-1}Ap_{n-1} = Ar_n - \frac{\beta_{n-1}}{\alpha_{n-1}}(r_n - r_{n-1}).$$

We then return to the formula for r_{n+1} to find

$$\begin{aligned}r_{n+1} &= r_n - \alpha_n w_n \\ &= r_n - \alpha_n Ar_n + \frac{\alpha_n\beta_{n-1}}{\alpha_{n-1}}(r_n - r_{n-1}).\end{aligned}$$

(iii) From the update formula for β_0, we have $\sqrt{\beta_0} = \frac{\|r_1\|}{\|r_0\|}$. Therefore $\delta + 0 = \frac{\sqrt{\beta_0}}{\alpha_0} = \frac{\|r_1\|}{\alpha_0\|r_0\|}$. By part (i) $r_1 = r_1 - \alpha_0 Ar_0$. If we divide through by $\|r_1\|$ and multiply through by δ_0 we find

$$\begin{aligned}r_1 &= r_0 - \alpha_0 Ar_0 \\ q_1 &= \frac{r_0}{\|r_1\|}Ar_0 \\ \delta_0 q_1 &= \frac{r_0}{\alpha_0\|r_0\|} - \frac{1}{\|r_0\|}Ar_0 \\ &= \gamma_0 q_0 - Aq_0.\end{aligned}$$

Rearranging gives $Aq_0 = \gamma_0 q_0 - \delta_0 q_1$.

Note that from the algorithm, $\beta_{n-1} = \frac{\|r_n\|^2}{\|r_{n-1}\|^2}$ so $-\delta_{n-1} = -\frac{1}{\alpha_{n-1}}\frac{\|r_n\|}{\|r_{n-1}\|}$, $-\delta_n = -\frac{1}{\alpha_n}\frac{\|r_{n+1}\|}{\|r_n\|}$, and $\gamma_n = \frac{1}{\alpha_n} + \frac{\|r_n\|^2}{\alpha_{n-1}\|r_{n-1}\|^2}$. Using the identity in part (ii), we have

$$\begin{aligned}
r_{n+1} &= r_n - \alpha_n A r_n + \frac{\alpha_n\beta_{n-1}}{\alpha_{n-1}} r_n - \frac{\alpha_n\beta_{n-1}}{\alpha_{n-1}} r_{n-1} \\
&= r_n - \alpha_n A r_n + \frac{\alpha_n\|r_n\|^2}{\alpha_{n-1}\|r_{n-1}\|^2} r_n - \frac{\alpha_n\|r_n\|^2}{\alpha_{n-1}\|r_{n-1}\|^2} r_{n-1} \\
&= r_n - \alpha_n A r_n + \frac{\alpha_n\|r_n\|^2}{\alpha_{n-1}\|r_{n-1}\|^2} r_n + \alpha_n\|r_n\|(-\delta_{n-1}q_{n-1}).
\end{aligned}$$

Dividing through by $\alpha_n\|r_n\|$ gives

$$\begin{aligned}
\frac{r_{n+1}}{\alpha_n\|r_n\|} &= \left(\frac{1}{\alpha_n} + \frac{\|r_n\|^2}{\alpha_{n-1}\|r_{n-1}\|^2}\right) q_n - Aq_n - \delta_{n-1}q_{n-1} \\
\frac{\|r_{n+1}\|}{\|r_{n+1}\|}\frac{r_{n+1}}{\alpha_n\|r_n\|} &= \gamma_n q_n - Aq_n - \delta_{n-1}q_{n-1} \\
\delta_n q_{n+1} &= \gamma_n q_n - Aq_n - \delta_{n-1}q_{n-1}.
\end{aligned}$$

Rearranging gives $Aq_n = -\delta_{n-1}q_{n-1} + \gamma_n q_n - \delta_n q_{n+1}$ as desired.

(iv) By part (iii),

$$\begin{aligned}
AQ_n &= [Aq_0 \quad Aq_1 \quad \cdots \quad Aq_{n-1}] \\
&= [\gamma_0 q_0 - \delta_0 q_1 \quad -\delta_0 q_0 + \gamma_1 q_1 - \delta_1 q_2 \quad \cdots \quad -\delta_{n-2}q_{n-2} + \gamma_{n-1}q_{n-1} - \delta_{n-1}q_n].
\end{aligned}$$

We see that this is exactly Q_nT_n except in the last column, where we're missing a term of $-\delta_{n-1}q_ne_n^T$ since Q_n only goes up to q_{n-1}. Thus $AQ_n = Q_nT_n - \delta_{n-1}q_ne_n^T$.

(v) Applying Q_n^T on the left to both sides of part (iv) gives us

$$Q_n^TAQ_n = Q_n^TQ_nT_n - \delta_{n-1}Q_nq_ne_n^T = T_n$$

since the q_n are orthonormal.

B

Odd N values consistently perform worse than even values because odd values have an interval that straddles 0.5, so checking odd values of N ensures that even values will also meet the tolerance. With that, the lowest value of N that meets the required tolerance is $N = 100$.

The Matlab code is on my github, file HW2b: https://github.com/HaleyColgate/Math714

C

(a) We initialize the scheme with the first time step, $t = 0$, as all zeros which the edges continue on with for the Dirichlet conditions. The next time step uses an approximation of the first derivative $U_t(x_i, y_j) \approx \frac{1}{\delta t}(U_{ij}^1 - U_{ij}^0)$ so $U_{ij} = \delta t f(x_i)f(y_j)$ to account for the initial condition of $u_t = f(x)f(y)$. Following that, we have the 3-point second derivative formula and the 5-point Laplacian which gives

$$\frac{U_{ij}^{n+1} - 2U_{ij}^n + U_{ij}^{n-1}}{\delta t^2} = \frac{U_{i+1j}^n + U_{i-1j}^n + U_{ij+1}^n + U_{ij-1}^n - 4U_{ij}^n}{\delta x^2}.$$

Therefore our update rule is

$$U_{ij}^{n+1} = 2U_{ij}^n - U_{ij}^{n-1} + \frac{\delta t^2}{\delta x^2}(U_{i+1j}^n + U_{i-1j}^n + U_{ij+1}^n + U_{ij-1}^n - 4U_{ij}^n).$$

See Figure 1 and note the slope of 2. This method is second order. Error should be worst at the largest time value. The Matlab code is on my github, file HW2C: https://github.com/HaleyColgate/Math714

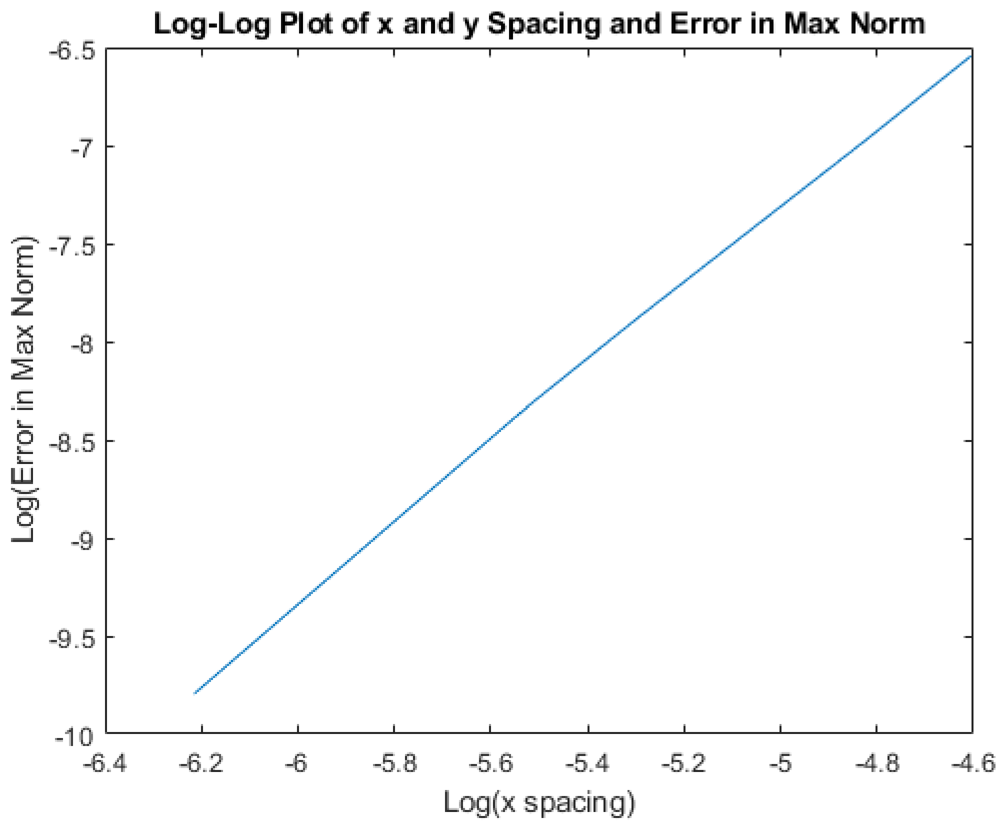

Figure 1: Log-Log Error Plot

(b) With the 3-point rule for y'' as a two step explicit time integrator we get the equation

$$\frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta t^2} = \lambda y_n$$

which simplifies to

$$0 = y_{n+1} - (\lambda \Delta t^2 + 2)y_n + y_{n-1}.$$

Our characteristic polynomial is then $\rho^2 - (\lambda \Delta t^2 + 2)\rho + 1$. We define $\alpha = \lambda \Delta t^2$ so $\rho = 1 + \frac{1}{2}\alpha \pm \sqrt{\frac{\alpha^2}{4} - 1}$. We need the magnitude of both values of ρ to be less than or equal to one, but as one gets smaller the other grows larger, so this happens only when they both have a magnitude of 1, for $-4 < \alpha < 0$.

(c) Our semi-discrete scheme is $y'' = \Delta_h y$ where $\Delta_h = I \otimes A + A \otimes I$ with

$$A = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & 0 \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ 0 & & & 1 & -2 \end{bmatrix}.$$

We know the kth eigenvalue of A is given by $\lambda_k(A) = -\frac{4}{h^2} \sin^2\left(\frac{k\pi h}{2}\right)$ for $k = 1, \ldots, N+1$ so as we've shown in the last homework

$$\lambda_{ij}(\Delta_h) = -\frac{4}{h^2} \sin^2\left(\frac{i\pi h}{2}\right) - \frac{4}{h^2} \sin^2\left(\frac{j\pi h}{2}\right).$$

We need $\lambda(\Delta_h)\delta t^2$ to be between -4 and 0 based on what we found in part (b). Conveniently, $\sin^2(i\pi h/2) + \sin^2(j\pi h/2)$ is bounded below by 0 and above by 2. We have

$$-4 < -\frac{4\Delta t^2}{h^2} \left(\sin^2\left(\frac{i\pi h}{2}\right) + \sin^2\left(\frac{j\pi h}{2}\right)\right) < 0$$

which simplifies to

$$0 < \frac{\Delta t^2}{h^2}\left(\sin^2\left(\frac{i\pi h}{2}\right) = \sin^2\left(\frac{j\pi h}{2}\right)\right) < 1.$$

With the bound on the sines this gives us $2\frac{\Delta t^2}{h^2} < 1$ or $\frac{\Delta t^2}{h^2} < \frac{1}{2}$.

(d) We suppose $U^n_{mj} = g(k_1, k_2)e^{ik_x mh}e^{ik_y jh}$ so $U^n = g(k_x, k_y)U^{n-1}$ so $U^{n+1} = g(k_x, k_y)^2 U_{n-1}$. For ease of notation from here forward $g = g(k_x, k_y)$. With our update rule this gives

$$e^{ik_x mh}e^{ik_y jh}g^2 = g\frac{\Delta t^2}{h^2}(e^{ik_x(m+1)h}e^{ik_y jh} + e^{ik_x(m-1)h}e^{ik_y jh} + e^{ik_x mh}e^{ik_y(j-1)h} + e^{ik_x mh}e^{ik_y(j+1)h}$$
$$+ \left(2\frac{h^2}{\Delta t^2} - 4\right)e^{ik_x mh}e^{ik_y jh}) - e^{ik_x mh}e^{ik_y jh}.$$

This simplifies to

$$g^2 = g\frac{\delta t^2}{h^2}\left(e^{ik_x h} + e^{-ik_x h} + e^{ik_y h} + e^{-ik_y h} + \left(2\frac{h^2}{\Delta t^2} - 4\right)\right) - 1$$

or

$$0 = g^2 - 2g\frac{\Delta t^2}{h^2}\left(\cos(k_x h) + \cos(k_y h) + \left(\frac{h^2}{\Delta t^2} - 2\right)\right) + 1.$$

Using the half angle formula $\cos(x) = 1 - 2\sin^2(x/2)$ and simplifying we get

$$\begin{aligned} 0 &= g^2 - 2g\frac{\Delta t^2}{h^2}(1 - 2\sin^2(k_x h/2) + 1 - 2\sin^2(k_y h/2) + (h^2/\Delta t^2 - 2)) + 1 \\ &= g^2 - 2g\frac{\Delta t^2}{h^2}(-2\sin^2(k_x h/2) - 2\sin^2(k_y h/2) + h^2/\Delta t^2) + 1 \\ &= g^2 + g\left(4\frac{\Delta t^2}{h^2}\sin^2\left(\frac{k_x h}{2}\right) + 4\frac{\Delta t^2}{h^2}\sin^2\left(\frac{k_y h}{2}\right) - 2\right) - 2. \end{aligned}$$

If we define

$$-\alpha = 4\frac{\Delta t^2}{h^2}\sin^2\left(\frac{k_x h}{2}\right) + 4\frac{\Delta t^2}{h^2}\sin^2\left(\frac{k_y h}{2}\right)$$

we find $0 = g^2 - (\alpha + 2)g - 2$ so $g = 1 + \frac{\alpha}{2} \pm \sqrt{\frac{\alpha^2}{4} - 1}$ and from part (a) we know $|g| \leq 1$ when $-4 < \alpha < 0$ and by part (c) this happens when $\frac{\Delta t^2}{h^2} < \frac{1}{2}$.