CS 714: Methods of Computational Mathematics I Homework 2 Submission

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(A) (a) w_1, w_2, \ldots, w_n are orthogonal i.e. $\langle w_i, w_j \rangle = 0, \forall i \neq j.$ $v \in \text{span}\{w_1, w_2, \ldots, w_n\}$. Therefore, we have

$$v = a_1 w_1 + a_2 w_2 + \ldots + a_n w_n \tag{1}$$

Now, we have,

$$\sum_{j=1}^{n} \frac{\langle v, w_{j} \rangle}{||w_{j}||^{2}} w_{j} = \sum_{j=1}^{n} \frac{\langle a_{1}w_{1} + a_{2}w_{2} + \dots + a_{n}w_{n}, w_{j} \rangle}{||w_{j}||^{2}} w_{j}$$

$$= \sum_{j=1}^{n} \frac{\langle a_{j}w_{j}, w_{j} \rangle}{||w_{j}||^{2}} w_{j} \qquad \text{(Since, } w_{1}, w_{2}, \dots, w_{n} \text{ are orthogonal)}$$

$$= \sum_{j=1}^{n} \frac{a_{j} \langle w_{j}, w_{j} \rangle}{||w_{j}||^{2}} w_{j}$$

$$= \sum_{j=1}^{n} \frac{a_{j} ||w_{j}||^{2}}{||w_{j}||^{2}} w_{j} = \sum_{j=1}^{n} a_{j}w_{j} = v$$
(2)

Hence proved:

$$v = \sum_{j=1}^{n} \frac{\langle v, w_j \rangle}{||w_j||^2} w_j \tag{3}$$

(b) $A \in \mathbb{R}^{N \times N}$ is symmetric.

 $n^* \leq N$ is the number of iterations to convergence.

 r_0, r_1, \ldots, r_n^* are the residuals of the CG iteration.

The aim is to create a A-orthogonal basis for $span\{r_0, r_1, \ldots, r_n\}$ for $n \leq n^* - 1$.

We use Gram-Schmidt orthogonalization procedure starts with $p_0 = r_0$, and

$$p_n = r_n - \sum_{j=0}^{n-1} \frac{\langle r_n, p_j \rangle_A}{\|p_j\|_A^2} p_j \quad \text{for } 1 \le n \le n^* - 1$$
 (4)

i The number of iterations to convergence n^* may be strictly smaller than N. This is possible because in case the solution which is a linear combination lies in the Krylov sub space of \mathcal{K}_N , meaning that it can be expressed using Krylov space \mathcal{K}_n where n < N. In that case the number of iterations to convergence (i.e. we find the exact solution and error/residual equals 0), n^* will be strictly smaller than N.

ii To prove by induction on n,

$$\langle p_n, p_j \rangle_A = 0 \quad \text{for } 0 \le j < n \le n^* - 1$$
 (5)

Base case: For n = 1, j can only be equal to 0. So, we have:

$$\langle p_{1}, p_{0} \rangle = p_{1}^{t} A p_{0}$$

$$= (r_{1} - \frac{\langle r_{1}, p_{0} \rangle_{A}}{||p_{0}||_{A}^{2}} p_{0})^{t} A p_{0}$$

$$= r_{1}^{t} A p_{0} - \frac{\langle r_{1}, p_{0} \rangle_{A}}{||p_{0}||_{A}^{2}} p_{0}^{t} A p_{0}$$

$$= r_{1}^{t} A p_{0} - \frac{\langle r_{1}, p_{0} \rangle_{A}}{||p_{0}||_{A}^{2}} ||p_{0}||_{A}^{2}$$

$$= \langle r_{1}, p_{0} \rangle_{A} - \langle r_{1}, p_{0} \rangle_{A} = 0$$
(6)

Inductive step: To show that for any $0 < n < n^* - 1$ if

$$\langle p_n, p_j \rangle_A = 0 \quad \text{for } 0 \le j < n < n^* - 1$$
 (7)

holds, then

$$\langle p_{n+1}, p_j \rangle_A = 0 \quad \text{for } 0 \le j < n+1 \le n^* - 1$$
 (8)

also holds.

Assuming equation (7) is true, we consider equation (8) when j = n, because for cases when $0 \le j < n$ we already know it is true from equation (7). Therefore, we have:

$$\langle p_{n+1}, p_{n} \rangle_{A} = p_{n+1}^{t} A p_{n}$$

$$= (r_{n+1}^{t} - \sum_{j=0}^{n} \frac{\langle r_{n+1}, p_{j} \rangle_{A}}{\|p_{j}\|_{A}^{2}} p_{j}^{t}) A p_{n}$$

$$= r_{n+1}^{t} A p_{n} - \sum_{j=0}^{n} \frac{\langle r_{n+1}, p_{j} \rangle_{A}}{\|p_{j}\|_{A}^{2}} p_{j}^{t} A p_{n}$$

$$= r_{n+1}^{t} A p_{n} - \sum_{j=0}^{n} \frac{\langle r_{n+1}, p_{j} \rangle_{A}}{\|p_{j}\|_{A}^{2}} \langle p_{n}, p_{j} \rangle_{A}$$

$$= \langle r_{n+1}, p_{n} \rangle_{A} - \frac{\langle r_{n+1}, p_{n} \rangle_{A}}{\|p_{n}\|_{A}^{2}} \langle p_{n}, p_{n} \rangle_{A}$$

$$= \langle r_{n+1}, p_{n} \rangle_{A} - \frac{\langle r_{n+1}, p_{n} \rangle_{A}}{\|p_{n}\|_{A}^{2}} \|p_{n}\|_{A}^{2} = 0$$
(9)

Note that in the above we make use of the fact that A is symmetric and also that equation (7) holds hence rendering A-induced inner product 0 for cases where $0 \le j < n$.

Since both the base case and the inductive step have been proved as true, by mathematical induction on n. Therefore,

$$\langle p_n, p_j \rangle_A = 0 \quad \text{for } 0 \le j < n \le n^* - 1$$
 (10)

(c) $A \in \mathbb{R}^{N \times N}$ is a symmetric positive definite matrix. \mathbb{R}^N has an orthonormal basis of eigenvectors $\phi_1, \phi_2, \dots, \phi_N$, such that:

$$A\phi_n = \lambda_n \phi_n$$
 and $\langle \phi_n, \phi_i \rangle = \delta_{ni}$ (11)

We also have:

$$\lambda_1 \le \lambda_2 \le \ldots \le \lambda_N \tag{12}$$

and $v, w \in \mathbb{R}^N$

Since, $\phi_1, \phi_2, \dots, \phi_N$ form an orthonormal basis for \mathbb{R}^N , therefore, we can have the following:

$$v = a_1 \phi_1 + a_2 \phi_2 + \ldots + a_N \phi_N w = b_1 \phi_1 + b_2 \phi_2 + \ldots + b_N \phi_N$$
 (13)

where, a_i 's and b_j 's are real coefficients.

i Before, we proceed for the proof, we notice that \mathbb{R}^N has an orthonormal basis of eigenvectors $\phi_1, \phi_2, \dots, \phi_N$. Therefore, we have the following:

$$\langle \phi_n, \phi_j \rangle = \delta_{nj} = \begin{cases} 1 & \text{if, } n = j \\ 0 & \text{if, } n \neq j \end{cases}$$
 (14)

We need to prove:

$$\langle Av, w \rangle = \sum_{n=1}^{N} \lambda_n \langle v, \phi_n \rangle \langle \phi_n, w \rangle$$
 (15)

Considering, the right hand side, we have:

$$\langle Av, w \rangle = \langle A(a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N), b_1\phi_1 + b_2\phi_2 + \dots + b_N\phi_N \rangle$$

$$= \langle a_1A\phi_1 + a_2A\phi_2 + \dots + a_NA\phi_N, b_1\phi_1 + b_2\phi_2 + \dots + b_N\phi_N \rangle$$

$$= \langle a_1\lambda_1\phi_1 + a_2\lambda_2\phi_2 + \dots + a_N\lambda_N\phi_N, b_1\phi_1 + b_2\phi_2 + \dots + b_N\phi_N \rangle$$
(Using equation 11 above)
$$= \lambda_1a_1(b_1\delta_{11} + b_2\delta_{12} + \dots + b_N\delta_{1N})$$

$$+ \lambda_2a_2(b_1\delta_{21} + b_2\delta_{22} + \dots + b_N\delta_{2N})$$

$$+ \dots$$

$$+ \lambda_Na_N(b_1\delta_{N1} + b_2\delta_{N2} + \dots + b_N\delta_{NN})$$
(Using equation 14 above)
$$= \lambda_1a_1(b_1 \times 1 + b_2 \times 0 + \dots + b_N \times 0)$$

$$+ \lambda_2a_2(b_1 \times 0 + b_2 \times 1 + \dots + b_N \times 0)$$

$$+ \dots$$

$$+ \lambda_Na_N(b_1 \times 0 + b_2 \times 1 + \dots + b_N \times 1)$$
(Using equation 14 above)
$$= \lambda_1a_1b_1 + \lambda_2a_2b_2 + \dots + \lambda_Na_Nb_N$$

Now considering the left hand side, we have:

$$\sum_{n=1}^{N} \lambda_{n} \langle v, \phi_{n} \rangle \langle \phi_{n}, w \rangle = \sum_{n=1}^{N} \lambda_{n} \langle a_{1}\phi_{1} + a_{2}\phi_{2} + \dots + a_{N}\phi_{N}, \phi_{n} \rangle \langle \phi_{n}, b_{1}\phi_{1} + b_{2}\phi_{2} + \dots + b_{N}\phi_{N} \rangle$$

$$= \sum_{n=1}^{N} \lambda_{n} a_{n} \delta_{nn} b_{n} \delta_{nn} \quad \text{(Using equation 14 above)}$$

$$= \sum_{n=1}^{N} \lambda_{n} a_{n} \times 1 \times b_{n} \times 1 \quad \text{(Using equation 14 above)}$$

$$= \sum_{n=1}^{N} \lambda_{n} a_{n} b_{n}$$

$$= \lambda_{1} a_{1} b_{1} + \lambda_{2} a_{2} b_{2} + \dots + \lambda_{N} a_{N} b_{N}$$

$$(17)$$

Therefore, from equation (16) and (17) we have proved that:

$$\langle Av, w \rangle = \sum_{n=1}^{N} \lambda_n \langle v, \phi_n \rangle \langle \phi_n, w \rangle$$
 (18)

ii We know that $A \in \mathbb{R}^{N \times N}$ is a symmetric positive definite matrix. Hence for any $x \in \mathbb{R}^N$ we have:

$$x^{t}Ax > 0$$

$$\implies \langle Ax, x \rangle > 0$$
(19)

Substituting $x = \phi_n$ in the equation above, where ϕ_n is an eigenvector corresponding to the orthonormal basis of \mathbb{R}^N , we have;

$$\langle A\phi_n, \phi_n \rangle > 0$$

 $\implies \langle \lambda_n \phi_n, \phi_n \rangle > 0$ (Using equation 11 above)
 $\implies \lambda_n \langle \phi_n, \phi_n \rangle > 0$
 $\implies \lambda_n ||\phi_n||^2 > 0$ (20)

Since, $||\phi_n||^2 > 0$, therefore $\lambda_n > 0$ for all admissible values of n. Hence, we have proved that:

$$\lambda_n > 0 \qquad \text{for } 1 \le n \le N$$
 (21)

iii Let us first compute $||v||^2$ as follows:

$$||v||^2 = \langle a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N, a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N \rangle$$

$$= a_1^2 + a_2^2 + \dots + a_N^2 \qquad \text{(Using equation 14 above and definition of inner product)}$$
(22)

Next, we compute $\langle Av, v \rangle$ as follows:

$$\langle Av, v \rangle = \langle A(a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N), a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N \rangle$$

$$= \langle a_1A\phi_1 + a_2A\phi_2 + \dots + a_NA\phi_N, a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N \rangle$$

$$= \langle a_1\lambda_1\phi_1 + a_2\lambda_2\phi_2 + \dots + a_N\lambda_N\phi_N, a_1\phi_1 + a_2\phi_2 + \dots + a_N\phi_N \rangle$$
(Using equation 11 above)
$$= a_1^2\lambda_1 + a_2^2\lambda_2 + \dots + a_N^2\lambda_N$$
(23)

Since, we know that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$, hence we can write the above equation as:

$$\lambda_{1}(a_{1}^{2} + a_{2}^{2} + \dots + a_{N}^{2}) \leq \langle Av, v \rangle \leq \lambda_{N}(a_{1}^{2} + a_{2}^{2} + \dots + a_{N}^{2})$$

$$\implies \lambda_{1}||v||^{2} \leq \langle Av, v \rangle \leq \lambda_{N}||v||^{2}$$
(24)

Note that we used equation (22) in solving the above inequality. Hence, we have proved that:

$$\lambda_1 ||v||^2 \le \langle Av, v \rangle \le \lambda_N ||v||^2 \tag{25}$$

iv We proceed as follows:

$$||Av|| = \sqrt{\langle Av, Av \rangle}$$

$$= \sqrt{\langle A(a_1\phi_1 + a_2\phi_2 + \ldots + a_N\phi_N), A(a_1\phi_1 + a_2\phi_2 + \ldots + a_N\phi_N) \rangle}$$

$$= \sqrt{\langle a_1A\phi_1 + a_2A\phi_2 + \ldots + a_NA\phi_N, a_1\phi_1 + a_2\phi_2 + \ldots + a_N\phi_N \rangle}$$

$$= \sqrt{\langle a_1\lambda_1\phi_1 + a_2\lambda_2\phi_2 + \ldots + a_N\lambda_N\phi_N, a_1\lambda_1\phi_1 + a_2\lambda_2\phi_2 + \ldots + a_N\lambda_N\phi_N \rangle}$$
(Using equation 11 above)
$$= \sqrt{a_1^2\lambda_1^2 + a_2^2\lambda_2^2 + \ldots + a_N^2\lambda_N^2}$$
(Using equations 11 and 14 above)
$$\leq \sqrt{\lambda_N^2(a_1^2 + a_2^2 + \ldots + a_N^2)}$$
(Using equation 12 above)
$$= \lambda_N \sqrt{a_1^2 + a_2^2 + \ldots + a_N^2}$$
(we have already proved $\lambda_N > 0$)
$$= \lambda_N ||v||$$
(Using equation 22)

Therefore, we have proved:

$$||Av|| \le \lambda_N ||v|| \tag{27}$$

(d) In the following derivation we will use the update formulae from the CG algorithm as presented in class.

$$p_{n+1} = r_{n+1} + \beta_n p_n$$

$$= p_n \beta_n + r_n - \alpha_n w_n$$

$$= p_n \beta_n + r_n - \alpha_n A p_n$$

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

$$= (1 + \beta_n) p_n - \alpha_n A p_n - \beta_{n-1} p_{n-1}$$
(28)

for $1 \le n \le n^* - 2$ (Proved)

(e) Let us assume that $A \in \mathbb{R}^{N \times N}$ is non-singular. Therefore $det(A) \neq 0$. Hence, A^{-1} exists. Also, we have $AA^{-1} = A^{-1}A = I_N$, where I_N is the corresponding identity matrix. And rank(A) = N, so A is full-rank. We have:

$$det(\lambda I_N - A) = a_0 + a_1 \lambda + a_2 \lambda^2 + \ldots + \lambda^N = p(\lambda)$$
(29)

where $p(\lambda)$ is a monic-polynomial of degree N and is known as the characteristic polynomial of A. By Cayley-Hamilton theorem we know that p(A) = 0. Hence, we have:

$$a_0 + a_1 A + a_2 A^2 + \dots + A^N = 0$$

$$\implies A^N = -(a_0 I + a_1 A + a_2 A^2 + \dots + a_{N-1} A^{N-1})$$
(30)

Hence, we have proved that A^N is a linear combination of $I, A, A^2, \dots A^{N-1}$.

(f) We have $\alpha \neq 0$ and Au = f

$$u = u + \alpha(f - Au) \tag{31}$$

Richardson iteration is defined by

$$u_{n+1} = u_n + \alpha(f - Au_n) \tag{32}$$

i We have:

$$e_n = u_n - u$$

$$\implies u = u_n - e_n \tag{33}$$

Then,

$$e_{n+1} = u_{n+1} - u = u_{n+1} - u_n + e_n$$

$$= u_n + \alpha (f - Au_n) - u_n + e_n$$

$$= \alpha (f - Au_n) + e_n$$

$$= \alpha (Au - Au_n) + e_n$$

$$= \alpha A(u - u_n) + e_n$$

$$= e_n - \alpha A(u_n - u) = e_n - \alpha Ae_n$$

$$= (I - \alpha A)e_n$$

$$\therefore e_{n+1} = (I - \alpha A)e_n \quad \text{(Proved)}$$

ii Let the eigenvalues of A be $\lambda_1, \lambda_2, \dots, \lambda_N$. Hence, we have the following:

$$||I - \alpha A|| = \max_{1 \le j \le N} |1 - \alpha \lambda_j| = \rho \tag{35}$$

Therefore, we can say:

$$e_{n+1} = (I - \alpha A)e_n$$

$$\implies ||e_{n+1}|| = ||(I - \alpha A)e_n||$$

$$\implies ||e_{n+1}|| \le ||(I - \alpha A)||||e_n|| \quad \text{(Using norm inequalities)}$$

$$\implies ||e_{n+1}|| \le \rho ||e_n|| \quad \text{(From equation above)}$$
(36)

iii We know $\alpha \neq 0$. Let us assume that the eigenvalues of A have the following order:

$$\lambda_1 \le \lambda_2 \qquad \le \dots \le \lambda_N$$

$$\implies 1 - \alpha \lambda_1 \ge 1 - \alpha \lambda_2 \quad \ge \dots \ge 1 - \alpha \lambda_N$$
(37)

Hence, we will have:

$$\rho = \max_{1 \le j \le N} |1 - \alpha \lambda_j|$$

$$= \max(|1 - \alpha \lambda_1|, |1 - \alpha \lambda_N|)$$
(38)

In order to find α that minimizes ρ , we plot the function ρ with α as the independent variable. In Figure 1, one can see that the value of ρ is minimized when α corresponds to the point marked as "star". We find that value of α by solving the two line equations as follows:

$$1 - \alpha \lambda_1 = -1 + \alpha \lambda_N$$

$$\implies 2 = \alpha(\lambda_1 + \lambda_N)$$

$$\implies \alpha = \frac{2}{(\lambda_1 + \lambda_N)}$$
(39)

Hence, $\alpha_{min} = \frac{2}{(\lambda_1 + \lambda_N)}$. Therefore in that case, we have:

$$\rho_{min} = 1 - \frac{2\lambda_1}{\lambda_1 + \lambda_N} = \frac{\lambda_N - \lambda_1}{\lambda_N + \lambda_1}$$

$$= \frac{\kappa - 1}{\kappa + 1}$$
(40)

We used $\kappa = \lambda_N/\lambda_1 \ge 1$.

Therefore, from the above equation, we can say that $\rho_{min} < 1$. Hence proved.

iv We have:

$$0 < c \le \lambda_1 \le \lambda_N \le C < \infty \tag{41}$$

and

$$\alpha = 2/(c+C) \tag{42}$$

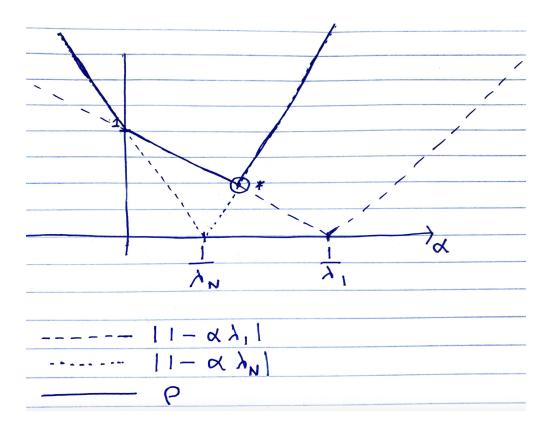


Figure 1: Plot of ρ vs. α

Therefore,

$$\rho = \max(|1 - \alpha \lambda_1|, |1 - \alpha \lambda_N|)$$

$$= \max(|1 - \frac{2\lambda_1}{c+C}|, |1 - \frac{2\lambda_N}{c+C}|)$$
(43)

We observe the following,

$$c \leq \lambda_{1} \qquad \leq C$$

$$\Rightarrow -2c \geq -2\lambda_{1} \qquad \geq -2C$$

$$\Rightarrow 1 - \frac{2c}{c+C} \geq 1 - \frac{2\lambda_{1}}{c+C} \qquad \geq 1 - \frac{2C}{c+C}$$

$$\Rightarrow \frac{C-c}{c+C} \geq 1 - \frac{2\lambda_{1}}{c+C} \qquad \geq \frac{c-C}{c+C}$$

$$\Rightarrow \frac{C-c}{c+C} \geq 1 - \frac{2\lambda_{1}}{c+C} \qquad \geq -\frac{C-c}{c+C}$$

$$\Rightarrow |1 - \frac{2\lambda_{1}}{c+C}| \leq \frac{C-c}{C+c}$$

$$\Rightarrow |1 - \frac{2\lambda_{1}}{c+C}| \leq \frac{C-c}{C+c}$$
(44)

Similarly, we can do for λ_N . Then from equation (43), we can say that:

$$\rho \le \frac{C - c}{C + c} = \frac{\kappa' - 1}{\kappa' + 1} \tag{45}$$

Again, since we assumed $\kappa' = C/c \ge 1$. Therefore, we have proved that:

$$\rho \le \frac{C - c}{C + c} = \frac{\kappa' - 1}{\kappa' + 1} < 1 \tag{46}$$

(g) We have

$$q_n = \frac{r_n}{\|r_n\|}$$
 for $0 \le n \le n^* - 1$ (47)

and $\{q_0, q_1, \ldots, q_{n-1}\}$ is an orthonormal basis for the Krylov space \mathcal{K}_n . In this part we will be using the update rules and formulae from the Conjugate Gradient algorithm presented in class.

i. We have:

$$r_1 = r_0 - \alpha_0 w_0$$

$$= r_0 - \alpha_0 A p_0$$

$$= r_0 - \alpha_0 A r_0 \qquad \text{(Since } p_0 = r_0\text{)}$$

$$(48)$$

ii. For $1 \le n \le n^* - 1$, where n^* is the number of steps to convergence, we have:

$$r_{n+1} = r_n - \alpha_n w_n$$

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

$$= r_n - \alpha_n A r_n - \alpha_n A \beta_{n-1} p_{n-1}$$

$$= r_n - \alpha_n A r_n - \alpha_n \beta_{n-1} A p_{n-1}$$

$$= r_n - \alpha_n A r_n - \alpha_n \beta_{n-1} w_{n-1}$$

$$= r_n - \alpha_n A r_n - \frac{\alpha_n \beta_{n-1}}{\alpha_{n-1}} (r_n - r_{n-1})$$
(49)

Hence, proved.

iii. We have:

$$r_{n+1} = r_n - \alpha_n A r_n + \frac{\alpha_n \beta_{n-1}}{\alpha_{n-1}} (r_n - r_{n-1}) \quad \text{for } 1 \le n \le n^* - 1$$
 (50)

$$r_1 = r_0 - \alpha_0 A r_0 \tag{51}$$

$$\gamma_0 = \frac{1}{\alpha_0} \quad \text{and} \quad \gamma_n = \frac{1}{\alpha_n} + \frac{\beta_{n-1}}{\alpha_{n-1}} \quad \text{for } 1 \le n \le n^* - 1$$
(52)

$$\delta_n = \frac{\sqrt{\beta_n}}{\alpha_n} \tag{53}$$

$$\beta_{n-1} = \frac{||r_n||^2}{||r_{n-1}||^2} \tag{54}$$

We also use other formulae from the Conjugate Gradient algorithm as and when required. We start with the left hand side as follows:

$$\gamma_{0}q_{0} - \delta_{0}q_{1} = \frac{1}{\alpha_{0}}q_{0} - \frac{\sqrt{\beta_{0}}}{\alpha_{0}}q_{1}
= \frac{1}{\alpha_{0}}(q_{0} - \sqrt{\beta_{0}}q_{1})
= \frac{1}{\alpha_{0}}(\frac{r_{0}}{||r_{0}||} - \sqrt{\beta_{0}}\frac{r_{1}}{||r_{1}||})
= \frac{1}{\alpha_{0}}(\frac{r_{0}}{||r_{0}||} - \sqrt{\beta_{0}}\frac{(r_{0} - \alpha_{0}Ar_{0})}{||r_{1}||})
= \frac{1}{\alpha_{0}}(\frac{r_{0}}{||r_{0}||} - \frac{(r_{0} - \alpha_{0}Ar_{0})}{||r_{0}||})
= \frac{1}{\alpha_{0}}(\frac{r_{0} - r_{0} + \alpha_{0}Ar_{0}}{||r_{0}||})
= A\frac{r_{0}}{||r_{0}||} = Aq_{0} \quad \text{(Hence, proved)}$$

Again for $1 \le n \le n^* - 1$, we start we the left hand side and proceed as follows:

(Used major substitutions from equation (54)

Used major substitutions from equation (54))
$$= \frac{1}{||r_n||} \left(-\frac{\beta_{n-1}}{\alpha_{n-1}} r_{n-1} + \left(\frac{1}{\alpha_n} + \frac{\beta_{n-1}}{\alpha_{n-1}} \right) r_n - \frac{r_{n+1}}{\alpha_n} \right)$$

$$= \frac{1}{||r_n||} \left(-\frac{\beta_{n-1}}{\alpha_{n-1}} (r_n + \alpha_{n-1} w_{n-1}) + \left(\frac{1}{\alpha_n} + \frac{\beta_{n-1}}{\alpha_{n-1}} \right) r_n - \frac{(r_n - \alpha_n w_n)}{\alpha_n} \right)$$

$$= \frac{1}{||r_n||} \left(r_n \left(\frac{1}{\alpha_n} + \frac{\beta_{n-1}}{\alpha_{n-1}} - \frac{\beta_{n-1}}{\alpha_{n-1}} \right) - \beta_{n-1} w_{n-1} - \frac{r_n}{\alpha_n} + w_n \right)$$

$$= \frac{1}{||r_n||} \left(r_n \left(\frac{1}{\alpha_n} \right) - \beta_{n-1} w_{n-1} - \frac{r_n}{\alpha_n} + w_n \right)$$

$$= \frac{1}{||r_n||} \left(w_n - \beta_{n-1} w_{n-1} \right)$$

$$= \frac{1}{||r_n||} \left(Ap_n - \beta_{n-1} w_{n-1} \right)$$

$$= \frac{1}{||r_n||} \left(A(r_n + \beta_{n-1} p_{n-1}) - \beta_{n-1} Ap_{n-1} \right)$$

$$= \frac{1}{||r_n||} \left(Ar_n + \beta_{n-1} Ap_{n-1} - \beta_{n-1} Ap_{n-1} \right)$$

$$= Aq_n \quad \text{(Hence proved)}$$
(56)

iv. We have $Q=\left[\begin{array}{ccc}q_0 & q_1 & \cdots & q_{n-1}\end{array}\right]\in\mathbb{R}^{N\times n},$ where Q is orthogonal. We also have:

$$T_{n} = \begin{bmatrix} \gamma_{0} & -\delta_{0} \\ -\delta_{0} & \gamma_{1} & -\delta_{1} \\ & \ddots & \ddots & \ddots \\ & -\delta_{n-3} & \gamma_{n-2} & -\delta_{n-2} \\ & & -\delta_{n-2} & \gamma_{n-1} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$(57)$$

where T_n is tridiagonal and $e_n = [0 \ 0 \ \dots \ 1]^T \in \mathbb{R}^n$

We start with the left hand side and use results from the previous parts as follows:

$$AQ_{n} = A[q_{0} \quad q_{1} \quad \dots \quad q_{n-1}]$$

$$= [Aq_{0} \quad Aq_{1} \quad \dots \quad Aq_{n-1}]$$

$$= [\gamma_{0}q_{0} - \delta_{0}q_{1} \quad -\delta_{0}q_{0} + \gamma_{1}q_{1} - \delta_{1}q_{2} \quad \dots \quad -\delta_{n-2}q_{n-2} + \gamma_{n-1}q_{n-1} - \delta_{n-1}q_{n}]$$
(58)

Now, looking at the above equation, we can see that except for the last term in the last column, the others can be potentially obtained using T_n . We have:

$$Q_n T_n = [q_0 \quad q_1 \quad \dots \quad q_{n-1}] T_n$$

= $[\gamma_0 q_0 - \delta_0 q_1 \quad -\delta_0 q_0 + \gamma_1 q_1 - \delta_1 q_2 \quad \dots \quad -\delta_{n-2} q_{n-2} + \gamma_{n-1} q_{n-1}]$ (59)

Now, if we look at $q_n e_n^T$, we can see that it results in a matrix which is all zeros except for the right most column, which is nothing but q_n . Therefore, we have:

$$q_n e_n^T = \begin{bmatrix} 0 & 0 & \dots & q_n \end{bmatrix} \tag{60}$$

Noting that δ_{n-1} is a scalar quantity, then from the above three equations, we can clearly conclude that:

$$AQ_n = Q_n T_n - \delta_{n-1} q_n e_n^T \tag{61}$$

Hence, proved.

v. First we note that the columns of Q_n are orthonormal vectors, hence Q_n is an orthogonal matrix. Hence, we have:

$$Q_n^T Q_n = I (62)$$

Now, we start by left-multiplying equation (61) by Q_n^T . We have:

$$Q_n^T A Q_n = Q_n^T Q_n T_n - \delta_{n-1} Q_n^T q_n e_n^T$$

$$= I T_n - \delta_{n-1} Q_n^T q_n e_n^T \qquad \text{(Using equation (62))}$$

$$= T_n - \delta_{n-1} Q_n^T q_n e_n^T$$

Next, we analyze the part $Q_n^Tq_n$. Note that the rows in Q_n^T are orthonormal vectors. Also note that q_n is a column vector and it is not present in one of the rows of Q_n^T . Since, we know that for two orthonormal vectors q_i and q_j when $i \neq j$, we have $q_i \cdot q_j = 0$ (Dot product). Therefore, it is easy to see that $Q_n^Tq_n = 0$. Therefore, we can write the above equation as:

$$Q_n^T A Q_n = T_n - \delta_{n-1} Q_n^T q_n e_n^T$$

$$= T_n - \delta_{n-1} 0$$

$$= T_n \quad \text{(Hence proved)}$$
(64)

(B) We have $f(x) = e^{-400(x-0.5)^2}$ for $x \in [0,1]$. We sample from a grid $x_j = jh$ where h = 1/N and $0 \le j \le N$. We have the interpolant of f computed from the N+1 samples of $f(x_j)$ and denote it by \hat{f} . We want to find the smallest value of N such that f differs from \hat{f} by at most 10^{-2} in the uniform norm. The code for the numerical solution is present in this Github repository.

Link: https://github.com/sourav-roni/Math714_Homework2

Note: The code for this question is present in the folder "QuestionB". It has a README.md which describes other details.

We take the following two step approach. In order to get a rough sense (which turns out to be very good) we start with finding the error with respect to a very fine grid with 100000 grid points. We check the error of the interpolant for this fine grid with values of N starting from 10 unless the error drops below the threshold and trying values of N differing by 5. With this approach we find that the minimum desired value of N is 100. In order to further justify our findings, we do a refined processing. This involves analyzing the derivative of the difference function between f and \hat{f} . Note that, for grid interval $[x_i, x_{i+1}]$, we can write down the interpolant as follows:

$$\frac{\hat{f}(x) - f(x_j)}{x - x_j} = \frac{f(x_{j+1}) - f(x_j)}{x_{j+1} - x_j}$$

$$\therefore \hat{f}(x) = f(x_j) + (x - x_j) \frac{f(x_{j+1}) - f(x_j)}{x_{j+1} - x_j}$$

$$= f(x_j) + (x - x_j) \frac{f(x_{j+1}) - f(x_j)}{h}$$
(65)

Next, we can define the difference/error function in the interval as:

$$g(x) = \hat{f}(x) - f(x) \tag{66}$$

The idea is to exploit the derivative of g's in all the intervals, find where the maximum error occurs for each interval and finally find the maximum among them and compare to the threshold. Note, when we say maximum, we are comparing the absolute values. We make use of Matlab functions "diff" and

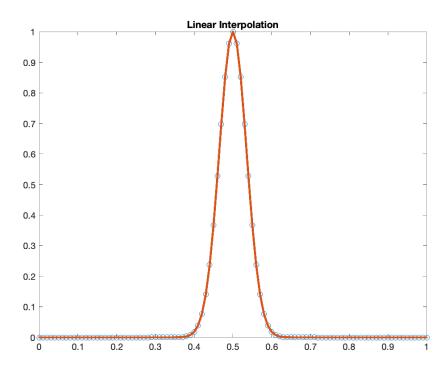


Figure 2: Linear interpolant

"fzero" to help us achieve the goal. We can see that the minimum value of N required is 100 in order to achieve the desired error bounds.

Note that the second step in the procedure defined above is computationally expensive, takes quite some time, hence to make the search more efficient we perform the first step and then use it as a cue for the second step.

Figure 2 shows the interpolant and the grid points for N = 100.

(C) We have the 2-D wave equation with homogeneous Dirichlet boundary conditions as follows:

$$u_{tt} = \Delta u, \qquad 0 \le x, y \le 1 \tag{67}$$

Initial conditions are given by:

$$u(x, y, 0) = 0,$$
 $u_t(x, y, 0) = f(x)f(y)$ (68)

where $f(x) = e^{-400(x-0.5)^2}$. We have $\mathbf{x}_j = (x_{j1}, y_{j2}) = (j_1 \Delta x, j_2 \Delta x)$ as spatial grid points.

(a) The implementation is present in this Github repository .

Link: https://github.com/sourav-roni/Math714_Homework2

Note: The code for this question is present in the folder "QuestionC". It has a README.md which describes other details.

The main equation that we use is as follows:

$$\frac{U_{i,j}^{n+1} - 2U_{i,j}^n + U_{i,j}^{n-1}}{(\Delta t)^2} = \frac{U_{i+1,j}^n + U_{i-1,j}^n + U_{i,j+1}^n + U_{i,j-1}^n - 4U_{i,j}^n}{h^2}$$
(69)

In the above equation, h is the spatial grid spacing. Coming to the initialization part, note that we know the grid values at t = 0 given by u(x, y, 0) = 0. As, it can be seen, that we still need the

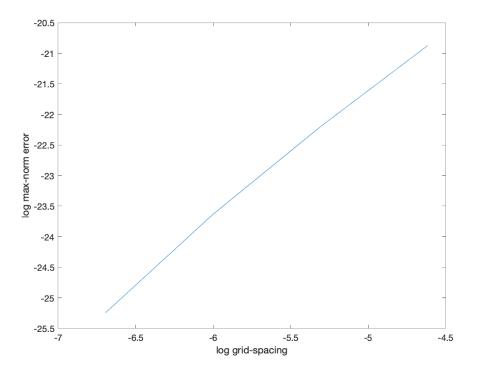


Figure 3: Log-log plot of error vs. the grid spacing

value at t = 1, after which we are able to use the formula above. In order to get that, we make use of the following:

$$\frac{U_{i,j}^{1} - U_{i,j}^{0}}{\Delta t} \approx u_{t}(x, y, 0) = f(x)f(y)$$

$$\Longrightarrow \frac{U_{i,j}^{1} - 0}{\Delta t} \approx f(x)f(y)$$

$$\therefore U_{i,j}^{1} \approx \Delta t f(x)f(y)$$
(70)

We use the above equation to get the values for the grid at t = 1. It is worth noting that the values at the boundary on both spatial dimensions remain zero throughout all instances of time. We make use of that fact in out implementation. The code presented also has additional comments that explain how we obtain the error plot making the use of a fine grid.

Figure 3 is the log-log error plot. Since the slope of the log-log plot of the error vs. the grid spacing Δx is close to 2 we can check from this plot that the method is second-order accurate.

(b) Here, we consider, $y''(t) = \lambda y$. Using the three point rule for y'', we end up with:

$$\rho - 2 + \frac{1}{\rho} = \lambda (\Delta t)^2$$

$$\implies \rho^2 - (2 + \lambda (\Delta t)^2)\rho + 1 = 0$$
(71)

The roots of the above quadratic equation are given by:

$$\rho = \frac{(2 + \lambda(\Delta t)^2) \pm \sqrt{(2 + \lambda(\Delta t)^2)^2 - 4}}{2}$$
 (72)

Let us assume $\theta = \lambda(\Delta t)^2$. Then we have the roots as:

$$\rho_{roots} = 1 + \frac{\theta}{2} \pm \sqrt{(1 + \frac{\theta}{2})^2 - 1} \tag{73}$$

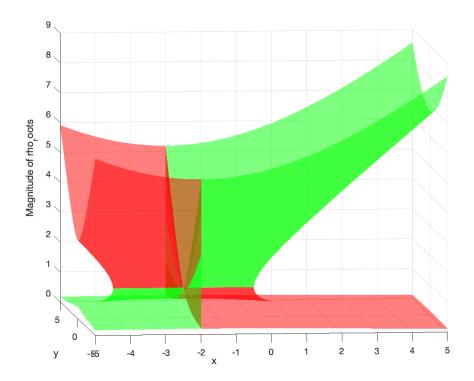


Figure 4: Plot of $|\rho_{roots}|$ vs. (x, y), where $\theta = x + iy$

We know that θ can be a complex number. Let us assume that $\theta = x + iy$. In order to find the region of stability we need to have a condition on θ such that $|\rho_{roots}| \leq 1$. To investigate the region of stability, we plot the values of $|\rho_{roots}|$ as a function of (x, y) where $\theta = x + iy$. The plot is presented in 4. Note that the green surface corresponds to the root obtained using the positive sign in equation (73) and the red surface corresponds to the one obtained using the negative sign in equation (73). The code for generating this plot is present in this Github repository under the folder of "QuestionC".

From Figure 4 we can conclude that in order for the magnitude of $\rho_{roots} \leq 1$, we would require the imaginary part of θ to be 0 and the real part of θ to be in between 0 and -4. Hence, when $\theta = x + iy$, we would require y = 0 and $-4 \leq x \leq 0$. Since, we have assumed $\theta = \lambda(\Delta t)^2$. Therefore, for region of stability we will have:

$$-4 \le \operatorname{Re}(\lambda(\Delta t)^2) \le 0$$
 and $\operatorname{Im}(\lambda(\Delta t)^2) = 0$ (74)

where, $\operatorname{Re}(\lambda(\Delta t)^2)$ refers to the real part and $\operatorname{Im}(\lambda(\Delta t)^2)$ refers to the imaginary part. Hence, the region of stability for the ODE solver in terms of $\lambda(\Delta t)^2$ is shown in the complex plane as a line segment in the interval [-4,0] on the real axis in Figure 5.

(c) In this part we perform "method of lines" stability analysis for the method in (a). We know, from previous knowledge that when we have :

$$A = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}_{(n \times n)}$$
 (75)

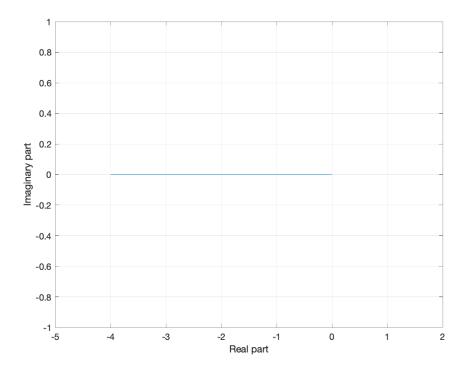


Figure 5: Region of stability in terms of $\lambda(\Delta t)^2$ in the complex plane

In the above equation n represents the number of grid points between 0 and 1. Note that we have the same grid spacing in both x and y dimensions and initial and boundary conditions are all zeros. Hence, we can write out the FD discretization only in terms of A as follows:

$$\Delta_h = A \otimes I + I \otimes A \tag{76}$$

where I is an identity matrix of appropriate dimensions. From our knowledge of the spectrum of the discrete Laplacian, we know that the eigenvalues of A are given by:

$$\lambda_k(A) = -\frac{4}{h^2} \sin^2(\frac{k\pi h}{2}); \qquad k = 1, \dots, N+1$$
 (77)

Also, in the previous homework, we have seen how to relate the eigenvalues of Δ_h to the eigenvalues of A and A (in this case). We note that the eigenvalues of Δ_h are all possible sums of the eigenvalues of A. Hence, they are given by:

$$\lambda_{k,l}(\Delta_h) = -\frac{4}{h^2}\sin^2(\frac{k\pi h}{2}) - \frac{4}{h^2}\sin^2(\frac{l\pi h}{2}); \qquad k,l \in \{1,\dots,N+1\}$$
 (78)

From the results of part(b) above, we know that for the stability region, we would require:

$$-4 \le \lambda_{k,l}(\Delta_h)(\Delta t)^2 \le 0$$

$$\implies -4 \le (\Delta t)^2 \left(-\frac{4}{h^2}\sin^2(\frac{k\pi h}{2}) - \frac{4}{h^2}\sin^2(\frac{l\pi h}{2})\right) \le 0 \quad \text{(Using equation above)}$$
(79)

We know that $\sin^2(x) \le 1$. So substituting the max value for $(\frac{4}{h^2}\sin^2(\frac{k\pi h}{2}) + \frac{4}{h^2}\sin^2(\frac{l\pi h}{2}))$ in the

above, we have:

$$-4 \le \frac{4(\Delta t)^2}{h^2}(-2) \le 0$$

$$\implies 0 \le \frac{4(\Delta t)^2}{h^2} \times 2 \le 4 \qquad \text{(Note: The LHS is always true)}$$

$$\therefore \frac{4(\Delta t)^2}{h^2} \times 2 \le 4$$

$$\implies \frac{(\Delta t)^2}{h^2} \le \frac{1}{2}$$
(80)

Therefore, the "method of lines" stability analysis results in the CFL conditions of $\frac{(\Delta t)^2}{h^2} \leq \frac{1}{2}$

(d) In this part we will perform Von Neumann stability analysis for the method in (a). We use $h = \Delta x$. For 2D wave equation, we have:

$$U_{i,j}^{n-1} = e^{ik_1ih}e^{ik_2jh}$$

$$U_{i,j}^n = g(k_1, k_2)e^{ik_1ih}e^{ik_2jh}$$

$$U_{i,j}^{n+1} = g(k_1, k_2)^2e^{ik_1ih}e^{ik_2jh}$$
(81)

Note: e stands for exponential and the first i in the power represents the imaginary number. From part (a), we have:

$$\frac{U_{i,j}^{n+1} - 2U_{i,j}^n + U_{i,j}^{n-1}}{(\Delta t)^2} = \frac{U_{i+1,j}^n + U_{i-1,j}^n + U_{i,j+1}^n + U_{i,j-1}^n - 4U_{i,j}^n}{h^2}$$
(82)

Now, we substitute values from equation (81) to equation (82) and write $g(k_1, k_2) = g$, to get:

$$\frac{g^2 e^{ik_1 ih} e^{ik_2 jh} - 2g e^{ik_1 ih} e^{ik_2 jh} + e^{ik_1 ih} e^{ik_2 jh}}{(\Delta t)^2} = \frac{g(e^{ik_1(i+1)h} e^{ik_2 jh} + e^{ik_1(i-1)h} e^{ik_2 jh} + e^{ik_1 ih} e^{ik_2(j+1)h} + e^{ik_1 ih} e^{ik_2(j-1)h} - 4e^{ik_1 ih} e^{ik_2 jh})}{h^2}$$

$$\Rightarrow (g^2 - 2g + 1) e^{ik_1 ih} e^{ik_2 jh} = \frac{(\Delta t)^2}{h^2} g e^{ik_1(i-1)h} e^{ik_2(j-1)h} [e^{ik_1 2h} e^{ik_2 h} + e^0 e^{ik_2 h} + e^{ik_1 h} e^{ik_2 2h} + e^{ik_1 h} e^0 - 4e^{ik_1 h} e^{ik_2 h}]$$

$$\Rightarrow (g^2 - 2g + 1) e^{ik_1 h} e^{ik_2 h} = \frac{(\Delta t)^2}{h^2} g [e^{ik_1 2h} e^{ik_2 h} + e^{ik_2 h} + e^{ik_1 h} e^{ik_2 2h} + e^{ik_1 h} - 4e^{ik_1 h} e^{ik_2 h}]$$

$$\Rightarrow (g^2 - 2g + 1) = \frac{(\Delta t)^2}{h^2} g [e^{ik_1 h} + e^{-ik_1 h} + e^{ik_2 h} + e^{-ik_2 h} - 4]$$

$$\Rightarrow (g^2 - 2g + 1) = \frac{(\Delta t)^2}{h^2} g [2\cos(k_1 h) + 2\cos(k_2 h) - 4]$$

$$\Rightarrow (g^2 - 2g + 1) = \frac{(\Delta t)^2}{h^2} g [2(1 - 2\sin^2(\frac{k_1 h}{2})) + 2(1 - 2\sin^2(\frac{k_2 h}{2})) - 4]$$

$$\Rightarrow (g^2 - 2g + 1) - \frac{(\Delta t)^2}{h^2} g [-4\sin^2(\frac{k_1 h}{2}) + 4\sin^2(\frac{k_2 h}{2})] = 0$$

$$\Rightarrow g^2 + g(-2 + \frac{(\Delta t)^2}{h^2} [4\sin^2(\frac{k_1 h}{2}) + 4\sin^2(\frac{k_2 h}{2})]) + 1 = 0$$

The roots of the above quadratic equation are given by:

$$g_{root} = \frac{2 - \frac{(\Delta t)^2}{h^2} \left[4\sin^2(\frac{k_1 h}{2}) + 4\sin^2(\frac{k_2 h}{2})\right] \pm \sqrt{\left(2 - \frac{(\Delta t)^2}{h^2} \left[4\sin^2(\frac{k_1 h}{2}) + 4\sin^2(\frac{k_2 h}{2})\right]\right)^2 - 4}}{2}$$
(84)

Let us use $\alpha = -\frac{(\Delta t)^2}{h^2} [4\sin^2(\frac{k_1h}{2}) + 4\sin^2(\frac{k_2h}{2})]$. Hence, we have:

$$g_{root} = \frac{2 + \alpha \pm \sqrt{(2 + \alpha)^2 - 4}}{2}$$

$$g_{root} = 1 + \frac{\alpha}{2} \pm \sqrt{(1 + \frac{\alpha}{2})^2 - 1}$$
(85)

The above equation is exactly the same as obtained in part(b) of this problem (equation(73)). Also, in this case for stability we would require the similar condition of $|g_{root}| \leq 1$. Hence, using the results from part(b) above, we have:

$$-4 \le -\frac{(\Delta t)^2}{h^2} \left[4\sin^2(\frac{k_1h}{2}) + 4\sin^2(\frac{k_2h}{2}) \right] \le 0$$

$$\implies 0 \le \frac{(\Delta t)^2}{h^2} \left[4\sin^2(\frac{k_1h}{2}) + 4\sin^2(\frac{k_2h}{2}) \right] \le 4$$
(86)

Since, we know $\sin^2(x) \le 1$, we substitute the maximum values in the above equation and have:

$$0 \le 4 \frac{(\Delta t)^2}{h^2} [2] \le 4$$

$$\implies 0 \le \frac{(\Delta t)^2}{h^2} \le \frac{1}{2}$$
(87)

Hence, the Von Neumann stability analysis results in the same CFL conditions as the previous part which is $\frac{(\Delta t)^2}{h^2} \leq \frac{1}{2}$.

(e) In this part we find the modified equation corresponding to the numerical method in (a). From part (a) we have:

$$\frac{U_{i,j}^{n+1} - 2U_{i,j}^n + U_{i,j}^{n-1}}{(\Delta t)^2} = \frac{U_{i+1,j}^n + U_{i-1,j}^n + U_{i,j+1}^n + U_{i,j-1}^n - 4U_{i,j}^n}{h^2}$$
(88)

Let us assume that the spacing in time is denoted by Δt and the grid spacing is denoted by $\Delta x = h$. Hence, we have:

$$U_{i,j}^{n} = u(x, y, t)$$

$$U_{i,j}^{n+1} = u(x, y, t + \Delta t)$$

$$U_{i,j}^{n-1} = u(x, y, t - \Delta t)$$

$$U_{i\pm 1,j}^{n} = u(x \pm h, y, t)$$

$$U_{i,j+1}^{n} = u(x, y \pm h, t)$$
(89)

Substituting values from equation (89) to equation (88), we have:

$$\frac{u(x,y,t+\Delta t) - 2u(x,y,t) + u(x,y,t-\Delta t)}{(\Delta t)^2}$$

$$= \frac{u(x+h,y,t) + u(x-h,y,t) + u(x,y+h,t) + u(x,y-h,t) - 4u(x,y,t)}{h^2}$$
(90)

The next step is to do Taylor series expansion on equation (90) and use the fact that $u_{tt} = u_{xx} + u_{yy}$.

That will lead us to the modified equation on which one can perform the Fourier analysis to comment on the physics of the extra terms and figure out whether they are dissipative, dispersive or something else.

Collaborators: Lewis Gross, Haley Colgate, Varun Gudibanda. We discussed the problems, however answers and code are my own.