MATH 5312 Advanced Numerical Methods II Final Project

Due date: 31 May, Wednsday

Answer all questions with reasoning.

1. Consider the finite difference discretization of the equation

$$\begin{cases} -(a(x)u'(x))' = f(x), & \text{for } x \in (0,1) \\ u(0) = u(1) = 0. \end{cases}$$

The discretized linear system is Au = f, where

$$\boldsymbol{A} = \begin{bmatrix} a_0 + a_1 & -a_1 \\ -a_1 & a_1 + a_2 & -a_2 \\ & -a_2 & a_2 + a_3 & -a_3 \\ & & \ddots & \ddots & \ddots \\ & & & -a_{n-2} & a_{n-2} + a_{n-1} & -a_{n-1} \\ & & & & -a_{n-1} & a_{n-1} + a_n \end{bmatrix}$$

and a_0, a_1, \ldots, a_n are a(x) on the grid points. Assume $C_1 \le a(x) \le C_2$ for all $x \in [0, 1]$, where C_1 and C_2 are positive constants.

- (a) Prove that \boldsymbol{A} is symmetric positive definite.
- (b) Show that both Jacobi and Gauss-Seidel converges for solving Au = f.
- (c) Prove that

$$4C_1\sin^2\left(\frac{\pi}{2(n+1)}\right) \le \lambda_1 \le \lambda_n \le 4C_2,$$

where λ_1 and λ_n are the smallest and largest eigenvalues of A respectively.

(d) Since \boldsymbol{A} is SPD, we may use the preconditioned conjugate gradient (PCG) to solve $\boldsymbol{A}\boldsymbol{u}=\boldsymbol{f}$. A candidate preconditioner will be

$$\mathbf{P} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Estimate the number of iterations needed for a solution with ϵ precision. Your answer should be as tight as possible. (This preconditioner will be practically useful for 2D case, because \mathbf{P} is diagonalizable by discrete sine transform and inverted very efficiently by fast Fourier transform.)

(a)
$$\forall x = (x_1, \dots, x_n)^T \in \mathbb{R}^n$$
. We have

$$\mathcal{A}^{T}AA = a_0 \mathcal{A}_1^{T} + \sum_{i=1}^{n-1} a_i (A_{i+1} - \mathcal{A}_i)^{T} + a_n \mathcal{A}_n^{T}$$

Note that C1 = a(x) = C2

then
$$0 = 0$$
 for $i = 0, 1, \dots, n \Rightarrow \pi^7 A \propto 20$

If AT AX =0.

Then
$$\forall \vec{v} = \begin{cases} 0 & \vec{v} = 1, \ \vec{v} = n \end{cases}$$

(b) · Jawbi:

Note that
$$2D-A = \begin{cases} a_0+a_1 & a_1 \\ a_1 & a_1+a_2 & a_2 \end{cases}$$

$$a_1 \quad a_1+a_2 \quad a_3 \quad a_4 \quad a_5 \quad \vdots \quad a_{n-1} \quad a_{n-1} + a_n$$

YZEIR7.

$$\chi^{7}(2D-A)\chi = Q_{0}\chi_{1}^{2} + \sum_{i=1}^{n-1} Q_{i}(\chi_{i} + \chi_{i-1})^{2} + Q_{n}\chi_{n}^{2} \ge 0$$

$$\chi^{7}(20-A)\chi = 0 \Leftrightarrow \chi = 0$$

· Gauss - Seidel:

Assume λ is the eigenvalue of G, and 3 is the corresponding eigenvector

$$\Rightarrow (1-(D-E)^{-1}A)3 = \lambda3$$

$$\Rightarrow \lambda = \frac{d - i\beta}{(\delta - d) - i\beta}$$

> 1 (8 - (d+ip)) = d-ip

$$\Rightarrow |\lambda|^2 = \frac{|\lambda|^2 + \beta^2}{(\delta - \lambda)^2 + \beta^2}$$

(c) For a unit vector
$$\chi \in \mathbb{R}^{n}$$
. $\chi = (\chi_{1}, \chi_{2}, ..., \chi_{n})^{7}$, $||\chi||_{1} = 1$
 $\chi^{7} A \chi = a_{0} \chi_{1}^{2} + \sum_{i=1}^{n-1} a_{i} (\chi_{i+1} - \chi_{i})^{2} + a_{n} \chi_{n}^{2}$

Note that
$$C_1 \leq G_1 \in C_2$$
 for $i = 0,1,...,n$

$$C_1 \left(\chi_1^2 + \sum_{i=1}^{n-1} (\chi_{i+1} - \chi_i^2)^2 + \chi_n^2\right) \leq \chi^T A \chi \leq C_2 \left(\chi_1^2 + \sum_{i=1}^{n-1} (\chi_{i+1} - \chi_i^2)^2 + \chi_n^2\right)$$

Denote
$$L = \begin{cases} 2 & -1 \\ -1 & 2 \end{cases}$$

Since
$$\lambda k(L) = 2(1-\omega s \frac{k}{n+1} \pi)$$
 $k=1,2,...,n$

Also, left hand side
$$2(1-\cos\frac{\pi}{n+1})=2.2\sin^3\frac{\pi}{2(n+1)}=4\sin^3\frac{\pi}{2(n+1)}$$

We have

$$4 \sin^{2} \frac{\pi}{2(n+1)} C_{1} \leq \pi^{T} A \pi \leq 4C_{2}$$

$$\Rightarrow 4C_{1} \sin^{2} \frac{\pi}{2(n+1)} \leq \lambda_{1} \leq \cdots \leq \lambda_{n} \leq 4C_{2}$$

(d)
$$P = d$$

$$\begin{pmatrix}
2 & -1 & & & \\
-1 & 2 & -1 & & \\
& & -1 & 2 & -1 & \\
& & & -1 & 2
\end{pmatrix}$$

$$\lambda \max (P^T A) \leq \lambda \max (P^T) \cdot \lambda \max (A) \leq \frac{C_L}{\lambda} \frac{\lambda \max (L)}{\lambda \min (L)}$$

$$\chi^T A \chi = \chi^T P P^T A \chi$$

Denote λ min (PTA) as the smallest eigenvalue of PTA, and A is the curresponding eigenvector.

$$\lambda \min (A) \leq \chi^T A \chi = \chi^T P \lambda \min (P^T A) \leq \lambda \max (P) \lambda \min (P^T A)$$

Amin
$$(P^{-1}A) \ge \frac{\lambda \min(A)}{\lambda \max(P)} \ge \frac{C_1}{\lambda} \frac{\lambda \min(L)}{\lambda \max(L)}$$

$$V \stackrel{\triangle}{=} \frac{\lambda_{max} (P^{-1}A)}{\lambda_{min} (P^{-1}A)} \leq \frac{C_2 \lambda_{max}^2 (L)}{C_1 \lambda_{min}^2 (L)} = \frac{C_2}{C_1 \tan^2 \frac{\pi}{2(nt)}}$$

When k<n

2 precision:

$$\Rightarrow k \geq O\left(\frac{\log \frac{1}{\xi} - \log \frac{1}{2||\chi_0 - \chi_{\star}||_{A}}}{\log \frac{\chi_{\star} - 1}{\chi_{\star} + 1}}\right)$$

Suppose & and 11 70 - 9x110 are constants.

$$\frac{\sqrt{r-1}}{\sqrt{r+1}} = \frac{\sqrt{c_2 - \sqrt{c_1} \tan \frac{\pi}{2(h+1)}}}{\sqrt{c_2} + \sqrt{c_1} \tan \frac{\pi}{2(h+1)}} = 1 - \sqrt{\frac{c_1}{c_1}} \tan \frac{\pi}{2(h+1)}$$

When kzn

2. The singular value decomposition (SVD) is a fundamental decomposition with numerous applications. In this question, we derive the SVD by the eigenvalue decomposition, and develop an algorithm for it. Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $m \geq n$. Since $\mathbf{A}^T \mathbf{A} \in \mathbb{R}^{n \times n}$ is square and symmetric positive semi-definite (SPSD), there exists an eigenvalue decomposition

$$A^T A = V \Lambda V^T.$$

where $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ are eigenvalues, and $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_n] \in \mathbb{R}^{n \times n}$ are corresponding eigenvectors.

- (a) Prove that $\mathbf{A}\mathbf{A}^T \in \mathbb{R}^{m \times m}$ has at most n nonzero eigenvalues, which are also $\lambda_1, \dots, \lambda_n$.
- (b) Therefore, $\mathbf{A}\mathbf{A}^T$ has an eigenvalue decomposition

$$AA^T = U\Lambda U^T.$$

where $U = [u_1, \dots, u_n] \in \mathbb{R}^{m \times n}$ are eigenvectors of AA^T corresponding to $\lambda_1, \dots, \lambda_n$ respectively. Assume all eigenvalues $\lambda_1, \dots, \lambda_n$ are all simple (though this assumption can be removed). Prove that there exists $\sigma_i \geq 0$, $i = 1, \dots, n$, such that

$$egin{cases} oldsymbol{A}oldsymbol{v}_i = \sigma_ioldsymbol{u}_i, \ oldsymbol{A}^Toldsymbol{u}_i = \sigma_ioldsymbol{v}_i, \ \sigma_i^2 = \lambda_i, \end{cases} i = 1, \ldots, n.$$

(c) Define $\sigma_i = \sqrt{\lambda_i}$, i = 1, ..., n. Prove that **A** has a decomposition

$$A = U\Sigma V^T$$
.

where $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$. This decomposition is SVD, and (σ_i, u_i, v_i) are called singular value, left and right singular vectors of \boldsymbol{A} respectively.

(d) Similar to eigenvalues of symmetric matrices, singular values also have many nice variational properties. Prove

$$\sigma_1 = \max_{\|\boldsymbol{u}\|_2 = 1, \|\boldsymbol{v}\|_2 = 1} \boldsymbol{u}^T \boldsymbol{A} \boldsymbol{v},$$

where σ_1 is the largest singular value of A. (There are other identities similar to the min-max theorem of eigenvalues.)

(e) Use (or not use) (d) to prove

$$\sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^T = \arg\min_{\mathrm{rank}(\boldsymbol{B})=1} \|\boldsymbol{A} - \boldsymbol{B}\|_F^2.$$

(That is, SVD gives the best rank-1 approximation. This can be extended to any best rank-r approximation, and this makes SVD a fundamental tool in many applications.)

(f) Propose a power iteration to compute the leading left and right singular vectors of \boldsymbol{A} . Your algorithm should use fewest possible matrix-vector products in each iteration. (All eigenvalue algorithms can be extended to SVD.)

(a)
$$A^{T}A = V \wedge V^{T}$$
. $A = diag(\lambda_{1}, \dots, \lambda_{n})$. $A \in \mathbb{R}^{m \times n}$, $m \ge n$

Consider matrix: $\begin{pmatrix} 0 & A \\ A^{T} & O \end{pmatrix}$

When $A \neq 0$

$$\begin{vmatrix} \lambda 1 - \begin{pmatrix} 0 & A \\ A^{T} & O \end{vmatrix} = \begin{vmatrix} \lambda 1 m & -A \\ -A^{T} & \lambda 1 n \end{vmatrix}$$

$$= \frac{1}{\lambda^{n}} \begin{vmatrix} \lambda 1 m & -A \\ -A^{T} & \lambda^{2} i n \end{vmatrix}$$

$$= \frac{1}{\lambda^{n}} \begin{vmatrix} \lambda^{2} m & -A A \\ -A^{T} & \lambda^{2} i n \end{vmatrix}$$

$$= \frac{1}{\lambda^{n}} \begin{vmatrix} \lambda^{2} 1 m & -AA A \\ -A^{T} & \lambda 1 n \end{vmatrix}$$

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$$= \frac{1}{\lambda^{n}} \begin{vmatrix} \lambda^{2} 1 m$$

Define
$$W_1 = AV_1$$
, $W_2 = AV_2$, ..., $W_n = AW_n$
Let $W = [W_1, ..., W_n] \in IR^{m_{XN}}$

Note that $V^{7}A^{7}AV = \Lambda \Rightarrow W^{T}W = \Lambda$ Define $Ui = \frac{WI}{\sqrt{\lambda i}} (\lambda i \neq 0)$

For $\lambda i = 0$. select orthornomal $u = Tu_1, \dots, u_n$ AVI = JAI UI Denote oi = shi. [= diag | 51, ..., 5n] AV=UΣ ⇒ uTA = IVT ⇒ ATU=VI ⇒ AT Ui = TUi In conclusion, (C) From (b) we have AV=UI Then, A=UIV7 (d) For UEIR MXM, I EIR MXM Define $\widetilde{\mathcal{U}} \in \mathbb{R}^{m_{XM}}$ as the completion of \mathcal{U} . û [, 1:n] =U. $\widehat{u}^{\mathsf{T}}\widetilde{u} = \widehat{u}\widetilde{u}^{\mathsf{T}} = 1$ Define $\widetilde{\Sigma} \in \mathbb{R}^{m \times n}$, $\widehat{\Sigma} = \begin{pmatrix} \Sigma \\ 0 \end{pmatrix}$ Then $A = U \Sigma V^{7} = \widetilde{U} \widetilde{\Sigma} V^{7}$ $\max_{\substack{\|\omega\|_{k}=1\\\|v\|_{k}=J\|}} u^{T}AV = \max_{\substack{\|\omega\|_{k}=J\\\|v\|_{k}=J\|}} u^{T} \widehat{u} \widehat{\xi} V V^{T}$ Since || Wut ||=|. || V VT ||=|. We can write RHS as || ulli=1 ut IVT $(u^{\intercal}\widehat{\Sigma}v^{\intercal})^{2} = (\sum_{i=1}^{n} \sigma_{i} u_{i} v_{i})^{2} \in (\sum_{i=1}^{n} u_{i}^{2}) (\sum_{i=1}^{n} \sigma_{i}^{2} v_{i}^{2}) = \sigma_{i}^{2}$ > u^T ~ v^T ≤ o => max uTAV = TI

Select u=u1, v=v1.

uitAVI = oi = oi wuld be achreved

Then $\widehat{u} = A^T V$

The leading right singular vector of A B V.

The leading left singular vector of A 13 U

3. We have used QR decomposition for solving the least squares (LS) problems in GMRES method

$$\min_{oldsymbol{x} \in \mathbb{R}^n} \|oldsymbol{A}oldsymbol{x} - oldsymbol{b}\|_2^2$$

where $\mathbf{A} \in \mathbb{R}^{m \times n}$ is rank r with $m \geq n$. Actually, LS problems arises in many other applications in applied mathematics and engineering, and there are other solvers for them. We consider to use the singular value decomposition (SVD) to solve LS problems.

(a) If we take only the non-zero singular values, then we obtain the compact SVD of \boldsymbol{A}

$$A = U\Sigma V^T$$
.

where $\boldsymbol{U} \in \mathbb{R}^{m \times r}$ satisfies $\boldsymbol{U}^T \boldsymbol{U} = \boldsymbol{I}$, $\boldsymbol{V} \in \mathbb{R}^{n \times r}$ satisfies $\boldsymbol{V}^T \boldsymbol{V} = \boldsymbol{I}$, and $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_r)$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$. Prove that

$$\operatorname{Ran}(\boldsymbol{A}) = \operatorname{Ran}(\boldsymbol{U}), \qquad \operatorname{Ker}(\boldsymbol{A}) = \operatorname{Ran}(\boldsymbol{V})^{\perp},$$

where $(\cdot)^{\perp}$ stands for the orthogonal complementary.

(b) Assume r = n. Prove that the solution of LS is unique and is given by

$$\boldsymbol{x} = \boldsymbol{V} \boldsymbol{\Sigma}^{-1} \boldsymbol{U}^T \boldsymbol{b}.$$

(c) Continuing (b): Let \tilde{x} be the solution of the LS when the input b is perturbed to \tilde{b} . Prove that

$$\frac{\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2}{\|\boldsymbol{x}\|_2} \le C \frac{\|\boldsymbol{b} - \tilde{\boldsymbol{b}}\|_2}{\|\boldsymbol{b}\|_2},$$

where $C = \frac{\sigma_1}{\sigma_n}$ if the LS is solved by formula in (b) and $C = \frac{\sigma_1^2}{\sigma_n^2}$ if the LS solution is obtained by solving the normal equation.

(d) Assume r < n. Prove that all solutions of LS are given by

$$x = V \Sigma^{-1} U^T b + y, \quad y \in \text{Ker}(A),$$

and $\boldsymbol{x}_0 := \boldsymbol{V} \boldsymbol{\Sigma}^{-1} \boldsymbol{U}^T \boldsymbol{b}$ is the solution of LS with the minimum 2-norm among all solutions.

(a) SVD decomposition of A:

⇒ Ran(A) I Ran(U)

> Ran (W) E Ran (A)

Hence Ran (A) = Ran (U)

$$A = U \Sigma V^{T} \implies Ran(V)^{L} = ker(V^{T}) \subseteq ker(A)$$

$$V^{T} = \Sigma^{-1} U^{T} A \implies ker(A) \subseteq ker(V^{T}) = Ran(V)^{L}$$

$$\implies ker(A) = Ran(V)^{L}$$

(b)
$$||A\chi - b||_{2}^{2} = ||U\Sigma V^{\perp} \chi - b||_{2}^{2}$$

= $||\Sigma V^{1} \chi - u^{7} b||_{2}^{2}$

(Let
$$y = V^{1} \pi$$
) = $\| \sum_{y} - u^{7} b \|_{2}^{2}$

Since min $|| \Sigma y - u^T b ||_2^2$ has a unique solution $y = \Sigma^T u^T b$ min $|| A \pi - b ||_2^2$ also has a unique solution $V^T \pi = \Sigma^T u^T b$ $\Rightarrow \pi = V \Sigma^T u^T b$

(c) •
$$\widetilde{x}$$
 is the solution of LS by the formula in (b) $\widetilde{x} = V \Sigma^{-1} u^{T} \widetilde{b}$

$$||x - \widehat{x}||_2 = ||V \Sigma^{-1} U^{7} (b - \widehat{b})||_2$$

$$\leq ||V \Sigma^{-1} U^{7} ||_2 ||b - \widehat{b}||_1$$

$$= || \sum_{i=1}^{n} ||_{2} ||_{b} - \widetilde{b} ||_{2}$$

Note that $\gamma = V \Sigma^{-1} u^{-1} b$

Thus 1/6/12 = 1/4 IV 7/12

Therefore,

•
$$\widetilde{\alpha}$$
 is the solution obtained by solving the normal equation $A^TAx = A^Tb \Rightarrow x = (A^TA)^TA^Tb$

$$A^T A \widehat{x} = A^T \widehat{b}$$
 \Rightarrow $\widehat{x} = (A^T A)^T A^T \widehat{b}$

$$\Rightarrow \frac{\|x-\widetilde{x}\|_{2}}{\|x\|_{2}} \leq \frac{\sigma^{2}}{|\sigma^{2}|} \frac{\|b-\widetilde{b}\|_{2}}{\|b\|_{2}}$$

(a)
$$\| A_{\pi} - b \|^2 = \| u \sum v^{7} \alpha - b \|^2$$

= $\| \widehat{u} \widehat{\Sigma} \widehat{V}^{7}_{\alpha} - b \|^2$

where $\widetilde{\mathcal{U}}$, $\widetilde{\Sigma}$, $\widetilde{\mathcal{V}}$ are full vectors and singular values with \mathcal{U} .

Solution:
$$Pr = \hat{\Sigma}^T D^T b$$

$$\Rightarrow \gamma = \widetilde{V}P = [Vr V_{n-r}) \begin{bmatrix} Pr \\ P_{n-r} \end{bmatrix}$$