Final Exam
CS383C/CAM383C/M383E

Take home. NO COLLABORATION. Do not consult anyone but me concerning this exam.

1. Consider the following level 3 BLAS implementation of the Modified Gramm-Schmidt method: Partition $m \times n$ matrix A and corresponding Q and R:

$$A = \left(\begin{array}{c|c} A_1 & A_2 \end{array} \right) = \left(\begin{array}{c|c} Q_1 & Q_2 \end{array} \right) \left(\begin{array}{c|c} R_{11} & R_{12} \\ \hline 0 & R_{22} \end{array} \right)$$

where A_1 is a $m \times b$ matrix.

- Factor $A_1 \to Q_1 R_{11}$.
- $R_{12} \leftarrow Q_1^T A_2$.
- $A_2 \leftarrow A_2 - Q_1 R_{12}$.
- Recursively continue with A_2.

(a) Which algorithm is this if $b = 1$?

(b) Using the Modified Gramm-Schmidt method to factor $A_1 \to Q_1 R_{11}$, what is the overall stability of this method compared to MGS and GS, when $b > 1$? (I am looking for an informal argument.)
Hint: Consider the following matrix:

$$\begin{pmatrix} 1 & 1 & 1 \\ \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{pmatrix}$$

Assume $\epsilon < \sqrt{\epsilon_{\text{mach}}}$ and that the only round-off error occurs when you compute $\text{fl}(\sqrt{1+\epsilon^2}) = 1$. Compute the QR factorization using Gramm-Schmidt, using Modified Gramm-Schmidt, and using the above algorithm with $b = 2$. [Comment added 12/12: Note: just by looking at what gets computed for this particular case you should be able to see a connection between CGS, MGS, and this blocked MGS, enough to answer the question.]

2. (a) **Note: the problem has been changed so that ther is no assumption about the columns of U being mutually orthogonal.**
Let $U = \left(\begin{array}{c|c|c|c} u_1 & u_2 & \cdots & u_k \end{array} \right) \in R^{m \times k}$ and $\{\beta_1, \cdots, \beta_k\} \in R$ Show that

$$(I + \beta_k u_k u_k^T)(I + \beta_{k-1} u_{k-1} u_{k-1}^T) \cdots (I + \beta_1 u_1 u_1^T) = (I + UTU^T)$$

where $k \times k$ matrix T is lower triangular.
Hint: Let $U_j = \left(\begin{array}{c|c|c|c} u_1 & u_2 & \cdots & u_j \end{array} \right)$. Assume that

$$(I + \beta_j u_j u_j^T)(I + \beta_{j-1} u_{j-1} u_{j-1}^T) \cdots (I + \beta_1 u_1 u_1^T) = (I + U_j T_j U_j^T)$$

Show that

$$\begin{aligned} & (I + \beta_{j+1} u_{j+1} u_{j+1}^T)(I + \beta_j u_j u_j^T) \cdots (I + \beta_1 u_1 u_1^T) \\ = \quad & I + \left(\begin{array}{c|c} U_j & u_{j+1} \end{array} \right) \left(\begin{array}{c|c} T_j & 0 \\ \hline x_{j+1}^T & \beta_{j+1} \end{array} \right) \left(\begin{array}{c|c} U_j & u_{j+1} \end{array} \right)^T \end{aligned}$$

for some vector x_{j+1}. (Note: this trick is used in blocked Householder transformation based QR factorization.)

3. Let $A \in R^{m \times n}$ be $m \times n$ have r linearly independent columns (rank$(A) = r$). We know that then its Singular Value Decomposition (SVD) can be given by $A = UDV^T$ where U is $m \times r$, D is $r \times r$ and diagonal, and V is $n \times r$. Moreover

$$U^T U = I, V^T V = I, \text{and } D = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma_r \end{pmatrix}$$

with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$.

   (a) Show the inverse: From basic principles, given U, V, and D with the above properties, show that A has rank r.

   (b) Show that the distance of A to the space of matrices of rank k (with $k < r$) is σ_{k+1}.
   Note: the distance of A to the space of matrices of rank k is defined by

$$\min_{E \text{ s.t. } rank(A+E)=k} \|E\|_2$$

(c) Show that for the Frobenius norm of A

$$\|A\|_F = \sqrt{\sigma_1^2 + \sigma_2^2 + \cdots + \sigma_r^2}$$

(Hint: Show that if Q is $n \times n$ and unitary ($Q^T Q = I$) then $\|QA\|_F = \|A\|_F$. Warning: U and V are NOT unitary, since they are not square. Thus you will have to think slightly deeper.)

For the remainder of the exam, go through the notes that I made regarding the QR algorithm and do the exercises marked with a $\star$.

Assumptions: [Note: ΛS changed to $S\Lambda$ on 12/12.]

$$AS = S\Lambda$$

where

- $$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

  with $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_{n-1}| > |\lambda_n|$. (Note: we are treating only a special case. Generalization is a bit messy, so we skip it.)

- S has linearly independent columns. In other words, A has simple eigenvalues.
- $$S = \begin{pmatrix} s_1 & s_2 & \cdots & s_n \end{pmatrix}$$
- $||s_i||_2 = 1$, $i = 1, \ldots, n$

Exercise 1 *Show that* $As_i = \lambda_i s_i$

1 Power Method

Given initial vector x iterate as follows:

- $x_0 = x$
- do $i = 0, \ldots$ until convergence
  - $\hat{x}_{i+1} = Ax_i$
  - $x_{i+1} = \hat{x}_{i+1}/\lambda_1$
- enddo

Exercise 2 *Show* $x = \alpha_1 s_1 + \cdots + \alpha_n s_n$. *(Hint:* $Sy = x$ *has a solution. How do* α_i*s relate to* y*?)*

Assume for the rest of the argument that $\alpha_1 \neq 0$. In other words, x has a component in the direction of s_1.

Exercise 3 *Show*

$$Ax = \alpha_1 \lambda_1 s_1 + \cdots + \alpha_n \lambda_n s_n$$

and

$$A^k x = \alpha_1 \lambda_1^k s_1 + \cdots + \alpha_n \lambda_n^k s_n$$

Exercise 4 *Show [Note: typo* s_n *changed to* s_2 *on 12/12]*

$$x_k = \alpha_1 s_1 + \alpha_2 \left(\frac{\lambda_2}{\lambda_1}\right)^k s_2 \cdots + \alpha_n \left(\frac{\lambda_n}{\lambda_1}\right)^k s_n$$

Exercise 5 ⋆ *Show*

$$||x_k - \alpha_1 s_1||_2 \leq (|\alpha_2| + \cdots + |\alpha_n|) \left(\frac{|\lambda_2|}{|\lambda_1|}\right)^k$$

and thus

$$||x_{k+1} - \alpha_1 s_1||_2 \leq \left(\frac{|\lambda_2|}{|\lambda_1|}\right) (|\alpha_2| + \cdots + |\alpha_n|) \left(\frac{|\lambda_2|}{|\lambda_1|}\right)^k$$

Notice that thus the bound on the difference between x_k and $\alpha_1 s_1$ (an eigenvector associated with λ_1) is decreased at each step by a factor $\frac{|\lambda_2|}{|\lambda_1|}$.

Practical Power Method:

- $x_0 = x$
- do $i = 0, \ldots$ until convergence
  - $\hat{x}_{i+1} = Ax_i$
  - $x_{i+1} = \hat{x}_{i+1} / ||\hat{x}_{i+1}||_2$
- enddo

2 Inverse Power Method

Given initial vector x iterate as follows:

- $x_0 = x$
- do $i = 0, \ldots$ until convergence
  - $\hat{x}_{i+1} = A^{-1} x_i$
  - $x_{i+1} = \lambda_n \hat{x}_{i+1}$
- enddo

Assume for the rest of the argument that $\alpha_n \neq 0$. In other words, x has a component in the direction of s_n.

Exercise 6 *Show*

$$A^{-1}x = \alpha_1 \frac{1}{\lambda_1} s_1 + \cdots + \alpha_n \frac{1}{\lambda_n} s_n$$

and

$$A^{-k}x = \alpha_1 \frac{1}{\lambda_1^k} s_1 + \cdots + \alpha_n \frac{1}{\lambda_n^k} s_n$$

Exercise 7 *Show [Note: typo s_n changed to s_2 on 12/12]*

$$x_k = \alpha_1 \left(\frac{\lambda_n}{\lambda_1}\right)^k s_1 + \alpha_2 \left(\frac{\lambda_n}{\lambda_2}\right)^k s_2 \cdots + \alpha_{n-1} \left(\frac{\lambda_n}{\lambda_{n-1}}\right)^k s_{n-1} + \alpha_n s_n$$

Exercise 8 ⋆ *Show*

$$||x_k - \alpha_n s_n||_2 \leq (|\alpha_1| + \cdots + |\alpha_{n-1}|) \left(\frac{|\lambda_n|}{|\lambda_{n-1}|}\right)^k$$

and thus

$$||x_{k+1} - \alpha_n s_n||_2 \leq \left(\frac{|\lambda_n|}{|\lambda_{n-1}|}\right) (|\alpha_1| + \cdots + |\alpha_{n-1}|) \left(\frac{|\lambda_n|}{|\lambda_{n-1}|}\right)^k$$

Notice that thus the bound on the difference between x_k and $\alpha_n s_n$ (an eigenvector associated with λ_n) is decreased at each step by a factor $\frac{|\lambda_n|}{|\lambda_{n-1}|}$.

3 Shifted Inverse Power Method

Let the shift $\sigma \neq \lambda_n$ and assume $|\lambda_1 - \sigma| \geq |\lambda_2 - \sigma| \geq \cdots \geq |\lambda_{n-1} - \sigma| > |\lambda_n - \sigma|$

Given initial vector x iterate as follows:

- $x_0 = x$
- do $i = 0, \ldots$ until convergence
  - $\hat{x}_{i+1} = (A - \sigma I)^{-1} x_i$
  - $x_{i+1} = (\lambda_n - \sigma)\hat{x}_{i+1}$
- enddo

Assume for the rest of the argument that $\alpha_n \neq 0$. In other words, x has a component in the direction of s_n.

Exercise 9 *Show* $(A - \sigma I)s_i = (\lambda_i - \sigma)s_i$

Exercise 10 *Show [Note: typo A^{-1} fixed on 12/12.]*

$$(A - \sigma I)^{-1} x = \alpha_1 \frac{1}{\lambda_1 - \sigma} s_1 + \cdots + \alpha_n \frac{1}{\lambda_n - \sigma} s_n$$

and

$$(A^{-1} - \sigma I)^k x = \alpha_1 \frac{1}{(\lambda_1 - \sigma)^k} s_1 + \cdots + \alpha_n \frac{1}{(\lambda_n - \sigma)^k} s_n$$

Exercise 11 ⋆ *Show [Note: typo s_n changed to s_2 on 12/12]*

$$x_k = \alpha_1 \left(\frac{\lambda_n - \sigma}{\lambda_1 - \sigma}\right)^k s_1 + \alpha_2 \left(\frac{\lambda_n - \sigma}{\lambda_2 - \sigma}\right)^k s_2 \cdots + \alpha_{n-1} \left(\frac{\lambda_n - \sigma}{\lambda_{n-1} - \sigma}\right)^k s_{n-1} + \alpha_n s_n$$

Exercise 12 *Show*

$$||x_k - \alpha_n s_n||_2 \leq (|\alpha_1| + \cdots + |\alpha_{n-1}|) \left(\frac{|\lambda_n - \sigma|}{|\lambda_{n-1} - \sigma|}\right)^k$$

and thus

$$||x_{k+1} - \alpha_n s_n||_2 \leq \left(\frac{|\lambda_n - \sigma|}{|\lambda_{n-1} - \sigma|}\right) (|\alpha_1| + \cdots + |\alpha_{n-1}|) \left(\frac{|\lambda_n - \sigma|}{|\lambda_{n-1} - \sigma|}\right)^k$$

Notice that thus the bound on the difference between x_k and $\alpha_n s_n$ (an eigenvector associated with λ_n) is decreased at each step by a factor $\frac{|\lambda_n - \sigma|}{|\lambda_{n-1} - \sigma|}$.

Notice that by picking $\sigma \approx \lambda_n$ this factor can be decreased essentially to $\frac{|\lambda_n - \sigma|}{|\lambda_{n-1} - \lambda_n|}$.

Note: one can dynamically pick σ by using $\sigma_i = \frac{x_i^T A x_i}{x_i^T x_i}$ (the Rayleigh quotient) at each step. This leads to the Rayleigh quotient iteration.

4 QR Algorithm

Note: we assume all matrices involved are real. Furthermore review the condistions regarding the eigenvalues before the section on the power method.

Consider the iteration

- $A_0 = A$
- do $i = 0, \ldots$ until convergence
  - $A_i \rightarrow Q_i R_i$
  - $A_{i+1} \leftarrow R_i Q_i$
- enddo

Exercise 13 *Show* $A_{i+1} = Q_i^T A_i Q_i$ *and* $A_{i+1} = Q_i^T Q_{i-1}^T \cdots Q_0^T A Q_0 \cdots Q_{i-1} Q_i$.

Exercise 14 ⋆ *Show* $A^{k+1} = \hat{Q}_k \hat{R}_k$ *where* $\hat{Q}_k = Q_0 Q_1 \cdots Q_k$ *and* $\hat{R}_k = R_k R_{k-1} \cdots R_0$.

Exercise 15 ⋆ *Let*

$$\hat{R}_k = \begin{pmatrix} \hat{\rho}_{11}^{(k)} & \hat{\rho}_{12}^{(k)} & \cdots & \hat{\rho}_{1n}^{(k)} \\ 0 & \hat{\rho}_{22}^{(k)} & \cdots & \hat{\rho}_{2n}^{(k)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \hat{\rho}_{nn}^{(k)} \end{pmatrix}$$

and

$$\hat{Q}_k = \begin{pmatrix} \hat{q}_1^{(k)} & \hat{q}_2^{(k)} & \cdots & \hat{q}_n^{(k)} \end{pmatrix}$$

Show $A^{k+1} e_1 = \hat{\rho}_{11}^{(k)} \hat{q}_1^{(k)}$

Thus, the first column of $\hat{Q}_k$ is in the same direction as the vector that results from performing the power methods with $x = e_1$.

Exercise 16 $\star$ *Show* $A^{-(k+1)} = \hat{R}_k^{-1}\hat{Q}_k^T$.

Exercise 17 $\star$ *Let*

$$\hat{R}_k^{-1} = \begin{pmatrix} \hat{\rho}_{11}^{(k)} & \hat{\rho}_{12}^{(k)} & \cdots & \hat{\rho}_{1n}^{(k)} \\ 0 & \hat{\rho}_{22}^{(k)} & \cdots & \hat{\rho}_{2n}^{(k)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \hat{\rho}_{nn}^{(k)} \end{pmatrix}$$

Show $e_n^T A^{-(k+1)} = \hat{\rho}_{nn}^{(k)}\hat{q}_n^{(k)\,T}$ *(Added 12/7: Notice that this means that* $(A^T)^{-(k+1)}e_n = \hat{\rho}_{nn}^{(k)}\hat{q}_n^{(k)}$*.)*

Conclude that the last column of $\hat{Q}_k$ converges to the eigenvector associated with the smallest eigenvalue of A. (Added 12/7: Wrong: the last column of $\hat{Q}_k$ converges to the eigenvector of A^T associated with the smallest (in absolute value) eigenvalue of A^T, which is also the smallest (in absolute value) eigenvalue of A.) [Note: this conclusion is just a statement. It is not part of the above exercise.]

Exercise 18 $\star$ *Assume Q is unitary. Assume x equals an eigenvector associated with $\lambda \in \lambda(A^T)$ (Note: the transpose was added here on 12/7) and assume $||x||_2 = 1$. Let q_n, the last column of Q have the property that $q_n = x + e$ where $||e||_2 \leq \epsilon$, some small number. Show that*

$$Q^T A Q = \left(\begin{array}{c|c} A_{11} & a_{12} \\ \hline a_{21}^T & \alpha_{22} \end{array}\right)$$

where $||a_{21}||_2$ is small and α_{22} is close to λ.

Exercise 19 *Conclude that if the last column of $\hat{Q}_k$ converges to an eigenvector associated with λ_n, then the (n,n) element of $\alpha_{nn}^{(k)}$ converges to λ_n.*