STAT 309: MATHEMATICAL COMPUTATIONS I
FALL 2013
PROBLEM SET 5

1. Consider an $n \times n$ tridiagonal matrix of the form

$$T_\alpha = \begin{bmatrix} \alpha & -1 & & & & \\ -1 & \alpha & -1 & & & \\ & -1 & \alpha & -1 & & \\ & & -1 & \alpha & -1 & \\ & & & -1 & \alpha & -1 \\ & & & & -1 & \alpha \end{bmatrix},$$

where $\alpha \in \mathbb{R}$ is a real parameter.

(a) Verify that the eigenvalues of T_α are given by

$$\lambda_j = \alpha - 2\cos(j\theta), \qquad j = 1, \dots, n,$$

where

$$\theta = \frac{\pi}{n+1}$$

and that an eigenvector associated with each λ_j is

$$\mathbf{q}_j = [\sin(j\theta), \sin(2j\theta), \dots, \sin(nj\theta)]^\mathsf{T}.$$

Under what condition on α does this matrix become positive definite?

(b) If an iterative method with iteration matrix B_α is convergent, we define its *asymptotic rate of convergence* as

$$\lim_{m\to\infty} \left(\frac{-\log\|B_\alpha^m\|_2}{m} \right)$$

Take $\alpha = 2$.

(i) Will the Jacobi iteration converge for this matrix? If so, what will its asymptotic rate of convergence be?

(ii) Will the Gauss-Seidel iteration converge for this matrix? If so, what will its asymptotic rate of convergence be?

(iii) For which values of ω will the SOR iteration converge?

2. In general, a *semi-iterative method* is one that comprises two steps:

$$\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)} + \mathbf{b} \qquad \text{(Iteration)}$$

and

$$\mathbf{y}^{(m)} = \sum_{k=0}^{m} \alpha_k^{(m)} \mathbf{x}^{(k)}. \qquad \text{(Extrapolation)}$$

As in the lectures, we will assume that $M = I - A$ with $\rho(M) < 1$ and that we are interested to solve $A\mathbf{x} = \mathbf{b}$ for some nonsingular matrix $A \in \mathbb{C}^{n\times n}$. Let

$$\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x} \qquad \text{and} \qquad \boldsymbol{\varepsilon}^{(m)} = \mathbf{y}^{(m)} - \mathbf{x}.$$

Date: November 26, 2013 (Version 1.2); due: 12 noon, December 9, 2013. Turn in your solutions to Kirsten Wellman in Eckhart 108. No late homeworks will be accepted.

(a) By considering what happens when $\mathbf{x}^{(0)} = \mathbf{x}$, show that it is natural to impose

$$\sum_{k=0}^{m} \alpha_k^{(m)} = 1 \tag{2.1}$$

for all $m \in \mathbb{N} \cup \{0\}$. Henceforth, we will assume that (2.1) is satisfied for all problems in this problem set.

(b) Show that for all $m \in \mathbb{N}$, we may write

$$\boldsymbol{\varepsilon}^{(m)} = P_m(M)\mathbf{e}^{(0)}$$

for some $P_m \in \mathbb{C}[x]$ with $\deg(P_m) = m$ and $P_m(1) = 1$.

(c) Hence deduce that a necessary condition for convergence is that

$$\lim_{m\to\infty} \|P_m(M)\|_2 < 1$$

where $\|\cdot\|_2$ is the spectral norm. Is this condition also sufficient?

(d) Consider the case when

$$\alpha_0^{(m)} = \alpha_1^{(m)} = \cdots = \alpha_m^{(m)} = \frac{1}{m+1}$$

for all $m \in \mathbb{N} \cup \{0\}$. Show that if a sequence (any sequence, not necessarily one generated as in (Iteration)) is convergent and

$$\lim_{k\to\infty} \mathbf{x}^{(k)} = \mathbf{x}$$

then

$$\lim_{m\to\infty} \mathbf{y}^{(m)} = \mathbf{x}.$$

Is the converse also true?

3. It is clear that in any semi-iterative method defined by some $M \in \mathbb{C}^{n\times n}$ with $\rho(M) < 1$, we would like to solve the problem

$$\min_{P\in\mathbb{C}[x],\ \deg(P)=m,\ P(1)=1} \|P(M)\|_2. \tag{3.2}$$

Note that in the lectures, we required the polynomial P to satisfy $P(0) = 1$. Here we use a different condition, $P(1) = 1$, motivated by Problem **2**(a).

(a) Show that if $m \geq n$, then a solution to (3.2) is given by

$$P_m(x) = \frac{x^{m-n}\det(xI - M)}{\det(I - M)}.$$

How do we know that the denominator is non-zero?

(b) From now on assume that M is Hermitian with minimum and maximum eigenvalues $\lambda_{\min}, \lambda_{\max} \in \mathbb{R}$. Define

$$\|f\|_\infty = \sup_{x\in[\lambda_{\min},\lambda_{\max}]} |f(x)|.$$

Emulating our discussions in the lectures, show that for $m = 0, 1, \ldots, n-1$, the solution to the relaxed problem

$$\min_{P\in\mathbb{C}[x],\ \deg(P)=m,\ P(1)=1} \|P\|_\infty \tag{3.3}$$

would yield an upper bound to (3.2).

(c) Again by emulating our discussions in the lectures, show that the solution to (3.3) for $\lambda_{\min} = -1$ and $\lambda_{\max} = +1$ is given by the Chebyshev polynomials,

$$C_m(x) = \begin{cases} \cos(m \cos^{-1}(x)) & -1 \le x \le 1, \\ \cosh(m \cosh^{-1}(x)) & x > 1, \\ (-1)^m \cosh(m \cosh^{-1}(-x)) & x < -1. \end{cases}$$

(d) Hence deduce that the solution to (3.3) for $\lambda_{\min} = a$ and $\lambda_{\max} = b$ is given

$$P_m(x) = \frac{C_m\left(\dfrac{2x - (b+a)}{b-a}\right)}{C_m\left(\dfrac{2 - (b+a)}{b-a}\right)}. \tag{3.4}$$

Note that this solves (3.3) for all $m \in \mathbb{N}$ and not just $m \le n-1$.

(e) Show that the solution in (d) is unique.

4. Let $M \in \mathbb{C}^{n \times n}$ be Hermitian with $\rho(M) = \rho < 1$. Moreover, suppose that

$$\lambda_{\min} = -\rho, \quad \lambda_{\max} = \rho.$$

(a) Show that the P_m's in (3.4) satisfy a three-term recurrence relation

$$C_{m+1}\left(\frac{1}{\rho}\right) P_{m+1}(x) = \frac{2x}{\rho} C_m\left(\frac{1}{\rho}\right) P_m(x) - C_{m-1}\left(\frac{1}{\rho}\right) P_{m-1}(x)$$

for all $m \in \mathbb{N}$.

(b) Show that the semi-iterative method with $\alpha_k^{(m)}$ given by the coefficient of P_m in (3.4) may be written as

$$\mathbf{y}^{(m+1)} = \omega_{m+1}(M\mathbf{y}^{(m)} - \mathbf{y}^{(m-1)} + \mathbf{b}) + \mathbf{y}^{(m-1)}$$

where $\omega_1 = 1$ and

$$\omega_{m+1} = \frac{2C_m(1/\rho)}{\rho C_{m+1}(1/\rho)}$$

for $m = 0, 1, 2, \dots$. This is a slightly different Chebyshev method where we choose the normalization (2.1) instead of $\alpha_m^{(m)} = 1$ in the lecture.

(c) Show that

$$\|P_m(M)\|_2 = \frac{1}{C_m(1/\rho)} = \frac{1}{\cosh(m\sigma)}$$

where $\sigma = \cosh^{-1}(1/\rho)$. Deduce that $\|P_m(M)\|_2$ is a strictly decreasing sequence for all $m = 0, 1, 2 \dots$.

(d) Show that

$$e^{-\sigma} = (\omega - 1)^{1/2}$$

where

$$\omega = \frac{2}{1 + \sqrt{1 - \rho^2}} \tag{4.5}$$

and deduce that

$$\|P_m(M)\|_2 = \frac{2(\omega - 1)^{m/2}}{1 + (\omega - 1)^m}.$$

(e) Hence show that $(\omega_m)_{m=0}^{\infty}$ is strictly decreasing for $m \ge 2$ and that

$$\lim_{m \to \infty} \omega_m = \omega.$$

5. Let $M \in \mathbb{C}^{n\times n}$ be nonsingular with $\rho(M) < 1$ and suppose we are interested in solving

$$M\mathbf{x} = \mathbf{b}. \tag{5.6}$$

(a) Show that SOR applied to the system

$$\begin{bmatrix} I & -M \\ -M & I \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{z} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{b} \end{bmatrix} \tag{5.7}$$

yields the following iterations

$$\begin{aligned} \mathbf{x}^{(m+1)} &= \omega(M\mathbf{z}^{(m)} - \mathbf{x}^{(m)} + \mathbf{b}) + \mathbf{x}^{(m)}, \\ \mathbf{z}^{(m+1)} &= \omega(M\mathbf{x}^{(m+1)} - \mathbf{z}^{(m)} + \mathbf{b}) + \mathbf{z}^{(m)}, \end{aligned}$$

for $m = 0, 1, 2, \dots$.

(b) Define the sequence of iterates $\mathbf{y}^{(m)}$ by

$$\mathbf{y}^{(m)} = \begin{cases} \mathbf{x}^{(k)} & \text{if } m = 2k, \\ \mathbf{z}^{(k)} & \text{if } m = 2k+1. \end{cases}$$

Show that the iterations obtained in (a) are exactly the iterations in Problem **4**(b). This shows that SOR applied to (5.7) is equivalent to Chebyshev applied to (5.6) but with $\omega_m = \omega$ for all $m \in \mathbb{N}$. Note that if ω is chosen to be the value in (4.5), then this is in fact the optimal SOR parameter.

6. Let $A \in \mathbb{R}^{n\times n}$ be symmetric positive definite and $\mathbf{b} \in \mathbb{R}^n$. As usual, we write

$$\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k. \tag{6.8}$$

We assume that $\mathbf{x}_0$ is initialized in some manner. In the lectures we assumed $\mathbf{x}_0 = \mathbf{0}$ and so $\mathbf{r}_0 = \mathbf{b}$ but we will do it a little more generally here. Consider the quadratic functional

$$\varphi(\mathbf{x}) = \mathbf{x}^\mathsf{T} A\mathbf{x} - 2\mathbf{b}^\mathsf{T}\mathbf{x}.$$

(a) Show that

$$\nabla\varphi(\mathbf{x}_k) = -2\mathbf{r}_k$$

and hence if $\mathbf{x}_* \in \mathbb{R}^n$ is a stationary point of φ, then

$$A\mathbf{x}_* = \mathbf{b}.$$

Show also that $\mathbf{x}_*$ must be a minimizer of φ.

(b) Consider an iterative method

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \tag{6.9}$$

where $\mathbf{p}_0, \mathbf{p}_1, \mathbf{p}_2, \dots$ are search directions to be chosen later. Show that if we want α_k so that the function $f : \mathbb{R} \to \mathbb{R}$,

$$f(\alpha) = \varphi(\mathbf{x}_k + \alpha\mathbf{p}_k)$$

is minimized, then we must have

$$\alpha_k = \frac{\mathbf{r}_k^\mathsf{T}\mathbf{p}_k}{\mathbf{p}_k^\mathsf{T} A\mathbf{p}_k}. \tag{6.10}$$

(c) Deduce that

$$\varphi(\mathbf{x}_{k+1}) - \varphi(\mathbf{x}_k) = -\frac{(\mathbf{r}_k^\mathsf{T}\mathbf{p}_k)^2}{\mathbf{p}_k^\mathsf{T} A\mathbf{p}_k}$$

and therefore $\varphi(\mathbf{x}_{k+1}) < \varphi(\mathbf{x}_k)$ as long as $\mathbf{r}_k^\mathsf{T}\mathbf{p}_k \neq 0$.

(d) Show that if we choose
$$\mathbf{p}_k = \mathbf{r}_k, \tag{6.11}$$
we obtain the steepest decent method discussed in the lectures.

(e) Let the eigenvalues of A be $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$ and $P \in \mathbb{R}[t]$. Show that
$$\|P(A)\mathbf{x}\|_A \leq \max_{1\leq i\leq n} |P(\lambda_i)| \|\mathbf{x}\|_A$$
for every $\mathbf{x} \in \mathbb{R}^n$. [*Hint:* $A \succ 0$ and so has an eigenbasis].

(f) Using (e) and $P_\alpha(t) = 1 - \alpha t$, show that if we have (6.11), then
$$\|\mathbf{x}_k - \mathbf{x}_*\|_A \leq \max_{1\leq i\leq n} |P_\alpha(\lambda_i)| \|\mathbf{x}_{k-1} - \mathbf{x}_*\|_A$$
for all $\alpha \in \mathbb{R}$.

(g) Using properties of Chebyshev polynomials, show that
$$\min_{\alpha\in\mathbb{R}} \max_{\lambda_n\leq t\leq\lambda_1} |1 - \alpha t| = \frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}$$
and hence deduce that
$$\|\mathbf{x}_k - \mathbf{x}_*\|_A \leq \frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} \|\mathbf{x}_{k-1} - \mathbf{x}_*\|_A.$$

7. In this problem, you are required to randomly generate *sparse* matrices and sparse symmetric matrices of specified *densities*, i.e., proportion of nonzero elements, [cf. `sprandn` and `sprandsym` in Matlab/Octave/Scilab]. Modify the diagonal elements of your sparse matrices so that they are diagonally dominant and do likewise so that your sparse symmetric matrices are positive definite.

(a) Implement Gaussian elimination with partial pivoting and Gauss-Seidel method. Compare their speeds and accuracies on a range of diagonally dominant matrices of varying dimensions and densities.

(b) Implement Cholesky factorization and steepest descent method. Compare their speeds and accuracies on a range of symmetic positive definite matrices of varying dimensions and densities.

(c) Comment on your findings in (a) and (b) with relevant numerical evidence presented in graphs and/or tables.