Scientific Computing Homework #2

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Problem 1. *Set up the linear least squares system* $A\mathbf{x} \cong \mathbf{b}$ *for fitting the model function* $f(t, \mathbf{x}) = x_1 t + x_2 e^t$ *to the three data points* $(1, 2), (2, 3), (3, 5)$.

Solution.

$$A\mathbf{x} = \begin{bmatrix} 1 & e \\ 2 & e^2 \\ 3 & e^3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cong \begin{bmatrix} 2 \\ 3 \\ 5 \end{bmatrix} = \mathbf{b}.$$

□

Problem 2. *Let* A *be an* $m \times n$ *matrix and* $\mathbf{b}$ *an* m*-vector.*

(a) Prove that a solution to the least squares problem $A\mathbf{x} \cong \mathbf{b}$ *always exists.*

(b) Prove that such a solution is unique if, and only if, $\operatorname{rank}(A) = n$.

Proof. (a)

Definition. *A continuous function* f *on an unbounded set* $S \subset \mathbb{R}^n$ *is said to be* coercive *if*

$$\lim_{\|\mathbf{x}\| \to \infty} f(\mathbf{x}) = +\infty,$$

i.e., for any constant M*, there is an* $r > 0$ *(depending on* M*) such that* $f(\mathbf{x}) \geq M$ *for any* $\mathbf{x} \in S$ *such that* $\|\mathbf{x}\| \geq r$.

Lemma. *Let* $S \in \mathbb{R}^n$ *be closed and unbounded, if* f *is coercive on* S*, then* f *has a global minimum over* S.

Proof of Lemma. Without loss of generality, assume $\mathbf{0} \in S$. Since f is coercive on S, we have

$$\exists r > 0 \text{ s.t. } \forall \mathbf{x} \in S, \|\mathbf{x}\| > r, \quad f(\mathbf{x}) \geq f(\mathbf{0}). \tag{1}$$

Consider the closed and bounded (hence compact) set $A = \{\mathbf{x} \in S : \|\mathbf{x}\| \leq r\}$, we know from Calculus the fact that a continuous function on a compact set has both maximum and minimum, therefore

$$\exists \mathbf{x}^* \in A, \text{ s.t. } \forall \mathbf{x} \in A, f(\mathbf{x}) \geq f(\mathbf{x}^*). \tag{2}$$

Combining (1) and (2) completes the proof, i.e.,

$$\exists \mathbf{x}^* \in S, \text{ s.t. } \forall \mathbf{x} \in S, f(\mathbf{x}) \geq f(\mathbf{x}^*).$$

□

Consider the function $\phi : \mathbb{R}^n \to \mathbb{R}$ given by

$$\phi(\mathbf{y}) = \|\mathbf{b} - \mathbf{y}\|_2.$$

ϕ is coercive on the closed and unbounded set $\operatorname{span}(A)$, applying the above lemma yields

$$\exists \mathbf{y}^* \text{ s.t. } \forall \mathbf{y} \in \operatorname{span}(A), \quad \phi(\mathbf{y}) \geq \phi(\mathbf{y}^*). \tag{3}$$

Let $\mathbf{y}^* = A\mathbf{x}^*$, from (3), we see that $\mathbf{x}^*$ is a solution to the least squares problem $A\mathbf{x} \cong \mathbf{b}$, i.e.,

$$\|\mathbf{b} - A\mathbf{x}^*\|_2 = \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2.$$

(b) Sufficiency: If $\mathrm{rank}(A) = n$, then $\forall \mathbf{y} \in \mathrm{span}(A)$, there exists a unique $\mathbf{x} \in \mathbb{R}^n$, s.t. $\mathbf{y} = A\mathbf{x}$. Therefore, the $\mathbf{x}^*$ constructed in the proof of (a) is unique.

Necessity: if $\mathrm{rank}(A) < n$, then $\exists \mathbf{z} \in \mathbb{R}^n$ s.t. $A\mathbf{z} = \mathbf{0}$. Thus

$$\|\mathbf{b} - A(\mathbf{x}^* + \mathbf{z})\|_2 = \|\mathbf{b} - A\mathbf{x}^*\|_2 = \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2,$$

which contradicts the uniqueness of $\mathbf{x}^*$.

□

Problem 3. *Determine the Householder transformation that annihilates all but the first entry of the vector* $\begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T$. *Specifically, if*

$$\left(I - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}\right)\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

what are the values of α *and* $\mathbf{v}$*?*

Solution. Let $\mathbf{a} = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T$, then

$$\alpha = -\mathrm{sign}(a_1)\|\mathbf{a}\| = -2,$$

and

$$\mathbf{v} = \mathbf{a} - \alpha\mathbf{e}_1 = \begin{bmatrix} 3 & 1 & 1 & 1 \end{bmatrix}^T.$$

□

Problem 4. *Suppose you want to annihilate the second component of a vector*

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

using a Givens rotation, but a_1 *is already zero.*

(a) Is it still possible to annihilate a_2 *with a Givens rotation? If so, specify an appropriate Givens rotation; if not, explain why.*

(b) Under these circumstances, can a_2 *be annihilated with an elementary elimination matrix? If so, how? If not, why?*

Solution. (a) It is possible to annihilate a_2 with a Givens rotation

$$G = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

(b) We cannot annihilate a_2 with an elementary elimination matrix, since adding any scalar multiple of a_1 to a_2 does not change a_2.

□

Problem 5. *(a) In the Gram-Schmidt procedure of Section 3.5.3, if we define the orthogonal projectors* $P_k = \mathbf{q}_k\mathbf{q}_k^T$, $k = 1, \ldots, n$, *where* $\mathbf{q}_k$ *is the kth column of* Q *in the resulting QR factorization, show that*

$$(I - P_k)(I - P_{k-1}) \cdots (I - P_1) = I - P_k - P_{k-1} - \cdots - P_1.$$

(b) Show that the classical Gram-Schmidt procedure is equivalent to

$$\mathbf{q}_k = (I - (P_1 + \cdots + P_{k-1}))\mathbf{a}_k,$$

(c) Show that the modified Gram-Schmidt procedure is equivalent to

$$\mathbf{q}_k = (I - P_{k-1}) \cdots (I - P_1)\mathbf{a}_k.$$

(d) *An alternative way to stablize the classical procedure is to apply it more than once (i.e., iterative refinement), which is equivalent to taking*

$$\mathbf{q}_k = (I - (P_1 + \cdots + P_{k-1}))^m \mathbf{a}_k,$$

where $m = 2$ is typically sufficient. Show that all three of these variations are mathematically equivalent (thought they may differ markedly in finite-precision arithmetic).

Solution. (a) First we compute $\forall i \neq j$,

$$P_i P_j = (\mathbf{q}_i \mathbf{q}_i^T)(\mathbf{q}_j \mathbf{q}_j^T) = \mathbf{q}_i(\mathbf{q}_i^T \mathbf{q}_j)\mathbf{q}_j^T = (\mathbf{q}_i^T \mathbf{q}_j)\mathbf{q}_i \mathbf{q}_j^T = 0(\mathbf{q}_i \mathbf{q}_j^T) = O,$$

where the fourth equality holds since $\mathbf{q}_i$'s are the columns of an orthogonal matrix.

Now we employ a simple induction on k.

(i) For $k = 1$, the conclusion clearly holds.

(ii) Suppose the conclusion holds for some k, then for $k + 1$, we have

$$\begin{aligned}(I - P_{k+1})(I - P_k) \cdots (I - P_1) &= (I - P_{k+1})(I - P_k - P_{k-1} - \cdots - P_1) \\ &= I - P_{k+1} - P_k - \cdots - P_1 + P_{k+1}(P_k + \cdots + P_1) \\ &= I - P_{k+1} - P_k - \cdots - P_1,\end{aligned}$$

therefore the conlusion holds for $k + 1$ as well.

(b) The definition of the classical Gram-Schmidt procedure yields

$$\mathbf{q}_k = \mathbf{a}_k - \sum_{j=1}^{k-1}(\mathbf{q}_j^T \mathbf{a}_k)\mathbf{q}_j = \mathbf{a}_k - \sum_{j=1}^{k-1}\mathbf{q}_j(\mathbf{q}_j^T \mathbf{a}_k) = \mathbf{a}_k - \sum_{j=1}^{k-1}(\mathbf{q}_j \mathbf{q}_j^T)\mathbf{a}_k = (I - (P_1 + \cdots + P_{k-1}))\mathbf{a}_k.$$

(c) The definition of the modified Gram-Schmidt procedure yields

$$\begin{aligned}&\mathbf{a}_k \leftarrow \mathbf{a}_k - \mathbf{q}_1^T \mathbf{a}_k \mathbf{q}_1 = (I - P_1)\mathbf{a}_k \\ &\mathbf{a}_k \leftarrow \mathbf{a}_k - \mathbf{q}_2^T \mathbf{a}_k \mathbf{q}_2 = (I - P_2)\mathbf{a}_k \\ &\cdots \\ &\mathbf{a}_k \leftarrow \mathbf{a}_k - \mathbf{q}_{k-1}^T \mathbf{a}_k \mathbf{q}_{k-1} = (I - P_{k-1})\mathbf{a}_k \\ &\mathbf{q}_k \leftarrow \mathbf{a}_k\end{aligned}$$

Therefore

$$\mathbf{q}_k = (I - P_{k-1}) \cdots (I - P_1)\mathbf{a}_k.$$

(d) The equivalence of (b) and (c) follows directly from (a). To show the equivalence of (b) and (d), apply a mathematical induction on m and use the following property of P_k:

$$P_i P_j = \begin{cases} P_i \text{ if } i = j; \\ O \text{ if } i \neq j. \end{cases}$$

□

Problem 6. *What are the eigenvalues and corresponding eigenvectors of the following matrix?*

$$\begin{bmatrix} 1 & 2 & -4 \\ 0 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

Solution.

$$\begin{aligned}\lambda_1 = 1, &\quad \mathbf{x}_1 = c\begin{bmatrix}1 & 0 & 0\end{bmatrix}^T; \\ \lambda_2 = 2, &\quad \mathbf{x}_2 = c\begin{bmatrix}2 & 1 & 0\end{bmatrix}^T; \\ \lambda_3 = 3, &\quad \mathbf{x}_3 = c\begin{bmatrix}-1 & 1 & 1\end{bmatrix}^T,\end{aligned}$$

where c is an arbitrary constant. □

Problem 7. *Is there any real value for the parameter α such that the matrix*

$$\begin{bmatrix} 1 & 0 & \alpha \\ 4 & 2 & 0 \\ 6 & 5 & 3 \end{bmatrix}$$

(a) Has all real eigenvalues?

(b) Has all complex eigenvalues with nonzero imaginary parts?

In each case, either give such a value for α or give a reason why none exists.

Solution. The characteristic polynomial of the above matrix is

$$p(\lambda) = -\lambda^3 + 6\lambda^2 + (6\alpha - 11)\lambda + 8\alpha + 6.$$

(a) One such value is $\alpha = 0$.

(b) There is no α such that the matrix has all complex eigenvalues with nonzero imaginary parts.

Lemma. *Let A be any real matrix, let λ be a complex eigenvalue of A with corresponding eigenvector $\mathbf{x}$, then $\bar{\lambda}$ is an eigenvalue with corresponding eigenvector $\bar{\mathbf{x}}$.*

Let $\lambda_1 = \alpha + \beta i$ be an eigenvalue, then from the above lemma, we know that $\lambda_2 = \bar{\lambda} = \alpha - \beta i$ is also an eigenvalue, $\lambda_3 = \lambda_1$ or $\lambda_3 = \lambda_2$, in either case, $\lambda_1 + \lambda_2 + \lambda_3$ is a complex number with nonzero imaginary parts, contradicting the fact that $\lambda_1 + \lambda_2 + \lambda_3 = 6$.

□

Problem 8. *If λ is an eigenvalue of an $n \times n$ matrix A, show that λ^2 is an eigenvalue of A^2.*

Proof. Let $\mathbf{x}$ be the eigenvector of A corresponding to λ, i.e., $A\mathbf{x} = \lambda\mathbf{x}$, therefore

$$A^2\mathbf{x} = A(\lambda\mathbf{x}) = \lambda A\mathbf{x} = \lambda^2\mathbf{x},$$

which shows that λ^2 is an eigenvalue of A^2 with eigenvector $\mathbf{x}$. □

Problem 9. *Suppose the $n \times n$ matrix A has the block upper triangular form*

$$A = \begin{bmatrix} A_{11} & A_{12} \\ O & A_{22} \end{bmatrix},$$

where A_{11} is $k \times k$ and A_{22} is $(n-k) \times (n-k)$.

(a) If λ is an eigenvalue of A_{11} with corresponding eigenvector $\mathbf{u}$, show that λ is an eigenvalue of A. (Hint: Find an $(n-k)-$vector $\mathbf{v}$ such that $\begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}$ is an eigenvector of A corresponding to λ.)

(b) If λ is an eigenvalue of A_{22} (but not of A_{11}) with corresponding eigenvector $\mathbf{v}$, show that λ is an eigenvalue of A. (Hint: Find a k-vector $\mathbf{u}$ such that $\begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}$ is an eigenvector of A corresponding to λ.)

(c) If λ is an eigenvalue of A with corresponding eigenvector $\begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}$, where $\mathbf{u}$ is a k-vector, show that λ is either an eigenvalue of A_{11} with corresponding eigenvector $\mathbf{u}$ or an eigenvalue of A_{22} with corresponding eigenvector $\mathbf{v}$.

(d) Combine the previous parts of this exercise to show that λ is an eigenvalue of A if, and only if, it is an eigenvalue of either A_{11} or A_{22}.

Proof. (a)

$$A\begin{bmatrix} \mathbf{u} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ O & A_{22} \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} A_{11}\mathbf{u} \\ \mathbf{0} \end{bmatrix} = \lambda\begin{bmatrix} \mathbf{u} \\ \mathbf{0} \end{bmatrix},$$

where $\mathbf{0}$ is the zero vector of dimension $n-k$.

Therefore λ is an eigenvalue of A.

(b)

$$A\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}A_{11} & A_{12}\\ O & A_{22}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}A_{11}\mathbf{u}+A_{12}\mathbf{v}\\ A_{22}\mathbf{v}\end{bmatrix} = \lambda\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix},$$

We need to choose a specific $\mathbf{u}$ so that the last equality holds.

$$A_{11}\mathbf{u}+A_{12}\mathbf{v} = \lambda\mathbf{u} \Rightarrow (A_{11}-\lambda I)\mathbf{u} = A_{12}\mathbf{v} \Rightarrow \mathbf{u} = (A_{11}-\lambda I)^{-1}A_{12}\mathbf{v},$$

The invertibility of $A_{11}-\lambda I$ is guaranteed by the fact that λ is not an eigenvalue of A_{11}. Therefore, λ is an eigenvalue of A with corresponding eigenvector $\begin{bmatrix}(A_{11}-\lambda I)^{-1}A_{12}\mathbf{v} & \mathbf{v}\end{bmatrix}^T$.

(c) Since λ is an eigenvalue of A with corresponding eigenvector $\begin{bmatrix}\mathbf{u} & \mathbf{v}\end{bmatrix}^T$, we have

$$A\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}A_{11} & A_{12}\\ O & A_{22}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}A_{11}\mathbf{u}+A_{12}\mathbf{v}\\ A_{22}\mathbf{v}\end{bmatrix} = \lambda\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix},$$

If $\mathbf{v}\neq\mathbf{0}$, then $A_{22}\mathbf{v}=\lambda\mathbf{v}$, and thus λ is an eigenvalue of A_{22} with corresponding eigenvector $\mathbf{v}$.

If $\mathbf{v}=\mathbf{0}$, then $A_{11}\mathbf{u}=\lambda\mathbf{u}$, and hence λ is an eigenvalue of A_{11} with corresponding eigenvector $\mathbf{u}$.

(d) The sufficiency follows from (a) and (b) while the necessity follows from (c).

□

Problem 10. *(a) What are the eigenvalues of the Householder transformation*

$$H = I - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}},$$

where $\mathbf{v}$ *is any nonzero vector?*

(b) What are the eigenvalues of the plane rotation

$$G = \begin{bmatrix}c & s\\ -s & c\end{bmatrix},$$

where $c^2+s^2=1$*?*

Solution. (a) The characteristic polynomial of H is

$$p(\lambda) = \det(H-\lambda I) = \det\left((1-\lambda)I - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}\right),$$

hence

$\lambda_1 = 1$ is an eigenvalue of multiplicity $n-1$;
$\lambda_2 = -1$ is an eigenvalue with corresponding eigenvector $\mathbf{v}$.

(b) The characteristic polynomial of G is

$$p(\lambda) = \det(G-\lambda I) = \begin{vmatrix}c-\lambda & s\\ -s & c-\lambda\end{vmatrix} = (c-\lambda)^2+s^2,$$

therefore $\lambda_1 = c+is$ is an eigenvalue of G with corresponding eigenvector $\begin{bmatrix}1 & i\end{bmatrix}^T$ and $\lambda_2 = c-is$ is an eigenvalue with corresponding eigenvector $\begin{bmatrix}i & 1\end{bmatrix}^T$.

□