Math 221 Homework 4

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Question 3.1

Proof. Let $A = [a_1, \ldots, a_n]$ and suppose $q_1, \ldots, q_j$ have already been computed with $q_k^T q_\ell = \delta_{k\ell}$. In classical Gram–Schmidt (CGS) the coefficients are $r_{ji} = q_j^T a_i$, and the residual after j steps is $a_i - \sum_{k=1}^{j} r_{ki} q_k$. In modified Gram–Schmidt (MGS) one updates the working vector by successively subtracting the same projections, so after j steps the working vector is

$$w_i^{(j)} = a_i - \sum_{k=1}^{j} r_{ki} q_k,$$

which is exactly the expression highlighted in the hint (there written as $q_i = a_i - \sum_{k=1}^{j} r_{ki} q_k$ after j updates). Because q_{j+1} is orthogonal to q_k for $k \leq j$, we have

$$r_{(j+1)i}^{\text{MGS}} = q_{j+1}^T w_i^{(j)} = q_{j+1}^T \left(a_i - \sum_{k=1}^{j} r_{ki} q_k \right) = q_{j+1}^T a_i = r_{(j+1)i}^{\text{CGS}}.$$

Thus for every $j < i$ the two formulas produce the same r_{ji} in exact arithmetic. It follows that the final residual $a_i - \sum_{k=1}^{i-1} r_{ki} q_k$ is the same in both methods, hence $r_{ii} = \|a_i - \sum_{k=1}^{i-1} r_{ki} q_k\|_2$ and $q_i = (a_i - \sum_{k=1}^{i-1} r_{ki} q_k)/r_{ii}$ are identical as well. Therefore CGS and MGS are mathematically equivalent in exact arithmetic. $\square$

Question 3.3

1. *Proof.* Consider the block system

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}.$$

It is equivalent to the two equations

$$r + Ax = b, \qquad A^T r = 0.$$

From the first, $r = b - Ax$. Substituting into the second gives the normal equations

$$A^T(b - Ax) = 0 \iff A^T Ax = A^T b.$$

Since $A \in \mathbb{R}^{m \times n}$ has full column rank with $m \geq n$, the matrix $A^T A$ is symmetric positive definite, so the normal equations have a unique solution x^*. This x^* is the unique minimizer of $\|Ax - b\|_2$, and with $r^* = b - Ax^*$ we have $A^T r^* = 0$. Hence (r^*, x^*) satisfies the block system. Conversely, any solution (r, x) of the block system satisfies $A^T Ax = A^T b$, so $x = x^*$ and $r = b - Ax^*$. Therefore the block system has a (unique) solution in which x is exactly the least–squares minimizer of $\|Ax - b\|_2$. $\quad\square$

2. *Proof.* Let $A \in \mathbb{R}^{m \times n}$ have full column rank with $m \geq n$ and consider the symmetric coefficient matrix

$$K = \begin{bmatrix} I_m & A \\ A^T & 0 \end{bmatrix}.$$

Take a full SVD $A = U\Sigma V^T$ with $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ orthogonal and $\Sigma \in \mathbb{R}^{m \times n}$ whose nonzero diagonal entries are $\sigma_1 \geq \cdots \geq \sigma_n > 0$. Using the orthogonal similarity $Q = \mathrm{diag}(U, V)$,

$$Q^T K Q = \begin{bmatrix} I_m & \Sigma \\ \Sigma^T & 0 \end{bmatrix} =: K_\Sigma,$$

so $\|K\|_2 = \|K_\Sigma\|_2$, $\|K^{-1}\|_2 = \|K_\Sigma^{-1}\|_2$, and $\kappa_2(K) = \kappa_2(K_\Sigma)$. The eigenvalues of K_Σ are the roots of

$$\det \begin{bmatrix} (1 - \lambda)I_m & \Sigma \\ \Sigma^T & -\lambda I_n \end{bmatrix} = \det\big((1 - \lambda)I_m\big) \det\left(-\lambda I_n - \Sigma^T\big((1 - \lambda)I_m\big)^{-1}\Sigma\right),$$

which for $\lambda \neq 1$ equals

$$(1 - \lambda)^{m-n} \det\big(\lambda(\lambda - 1)I_n - \Sigma^T\Sigma\big) = (1 - \lambda)^{m-n} \prod_{i=1}^{n}\big(\lambda^2 - \lambda - \sigma_i^2\big).$$

By continuity this is the characteristic polynomial. Hence the eigenvalues are

$$\lambda = 1 \text{ (with multiplicity } m - n), \qquad \lambda_{i,\pm} = \frac{1}{2}\left(1 \pm \sqrt{1 + 4\sigma_i^2}\right), \ i = 1, \ldots, n.$$

Since K_Σ is symmetric, its singular values are the absolute values of these eigenvalues. Therefore

$$\sigma_{\max}(K) = \max\left\{1, \max_i \tfrac{1}{2}\left(1 + \sqrt{1 + 4\sigma_i^2}\right)\right\} = \frac{1}{2}\left(1 + \sqrt{1 + 4\sigma_{\max}(A)^2}\right),$$

and

$$\sigma_{\min}(K) = \begin{cases} \min\left\{1, \tfrac{1}{2}\left(\sqrt{1 + 4\sigma_{\min}(A)^2} - 1\right)\right\}, & m > n, \\ \tfrac{1}{2}\left(\sqrt{1 + 4\sigma_{\min}(A)^2} - 1\right), & m = n. \end{cases}$$

Thus the 2–norm condition number $\kappa_2(K) = \sigma_{\max}(K)/\sigma_{\min}(K)$ is

$$\boxed{\kappa_2(K) = \frac{\tfrac{1}{2}\left(1 + \sqrt{1 + 4\sigma_{\max}(A)^2}\right)}{\min\left\{1, \tfrac{1}{2}\left(\sqrt{1 + 4\sigma_{\min}(A)^2} - 1\right)\right\}} \quad (m > n),}$$

and, when $m = n$,

$$\boxed{\kappa_2(K) = \frac{1 + \sqrt{1 + 4\sigma_{\max}(A)^2}}{\sqrt{1 + 4\sigma_{\min}(A)^2} - 1}.}$$

These expressions depend only on the extreme singular values of A and agree with the eigenvalue structure derived above. $\square$

3. *Proof.* Let $A \in \mathbb{R}^{m \times n}$ have full column rank and let

$$K = \begin{bmatrix} I_m & A \\ A^T & 0 \end{bmatrix}.$$

Since $A^T A$ is symmetric positive definite, we may form the 2×2 block LU factorization

$$K = \underbrace{\begin{bmatrix} I_m & 0 \\ A^T & I_n \end{bmatrix}}_{=:L} \underbrace{\begin{bmatrix} I_m & A \\ 0 & -A^T A \end{bmatrix}}_{=:U},$$

which is verified by direct multiplication. Both L and U are invertible with

$$L^{-1} = \begin{bmatrix} I_m & 0 \\ -A^T & I_n \end{bmatrix}, \qquad U^{-1} = \begin{bmatrix} I_m & -I_m \cdot A\,(-A^T A)^{-1} \\ 0 & (-A^T A)^{-1} \end{bmatrix} = \begin{bmatrix} I_m & A(A^T A)^{-1} \\ 0 & -(A^T A)^{-1} \end{bmatrix}.$$

Therefore $K^{-1} = U^{-1}L^{-1}$ and a single block multiplication yields

$$K^{-1} = \begin{bmatrix} I_m - A(A^T A)^{-1}A^T & A(A^T A)^{-1} \\ (A^T A)^{-1}A^T & -(A^T A)^{-1} \end{bmatrix}.$$

One easily checks that $K\,K^{-1} = K^{-1}K = I_{m+n}$, so the expression is the inverse. The $(2,1)$ block $(A^T A)^{-1}A^T$ is the familiar left pseudoinverse of A, which already appeared in the least–squares solution $x = (A^T A)^{-1}A^T b$. $\square$

3

4. *Proof.* Let $A \in \mathbb{R}^{m \times n}$ have full column rank and let $A = Q_1 R$ be a thin QR factorization, where $Q_1 \in \mathbb{R}^{m \times n}$ has orthonormal columns and $R \in \mathbb{R}^{n \times n}$ is upper triangular with positive diagonal. The least–squares solution minimizes $\|Ax - b\|_2$ and, in exact arithmetic, is $x_\star$ with $R x_\star = Q_1^T b$. Suppose $\hat{x}$ is a computed approximation. Define the residual $r = b - A\hat{x}$. The best correction δx is the minimizer of $\|A\delta x - r\|_2$, because $x_\star - (\hat{x} + \delta x)$ has residual $A(x_\star - \hat{x} - \delta x) = A\delta x - r$. Using $A = Q_1 R$ and orthogonality of Q_1, we have

$$\|A\delta x - r\|_2 = \|Q_1^T(A\delta x - r)\|_2 = \|R\delta x - Q_1^T r\|_2,$$

so the unique minimizer satisfies the triangular system

$$R\,\delta x = Q_1^T r.$$

The refined iterate is $\hat{x}^+ = \hat{x} + \delta x$. Repeating this with new residuals yields the iterative refinement scheme

$$r_k = b - A x_k, \qquad R\,\delta x_k = Q_1^T r_k, \qquad x_{k+1} = x_k + \delta x_k,$$

which uses only applications of Q_1^T (via Householder reflectors) and triangular solves with R. This update is also obtained by applying an orthogonal similarity to the block KKT system $K = \begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix}$: with $S = \mathrm{diag}(Q_1^T, I)$ one has $S^T K S = \begin{bmatrix} I & R \\ R^T & 0 \end{bmatrix}$, hence the correction for right–hand side $\begin{bmatrix} r_k \\ 0 \end{bmatrix}$ solves $R\,\delta x_k = Q_1^T r_k$ and produces the same $\hat{x}^+$. When the residual r_k is formed in higher precision and the QR solves are backward stable, the standard analysis of iterative refinement (cf. the linear system case) shows a reduced forward error for x_{k+1} compared with x_k. Thus a precomputed QR factorization furnishes an efficient and stable iterative refinement algorithm for improving the accuracy of the least–squares solution. $\qquad \square$

Question 3.4

Proof. Let $C \in \mathbb{R}^{m \times m}$ be symmetric positive definite and define the weighted least–squares objective

$$\phi(x) \;=\; \tfrac{1}{2}\|Ax - b\|_C^2 \;=\; \tfrac{1}{2}(Ax - b)^T C(Ax - b).$$

Differentiating gives $\nabla \phi(x) = A^T C(Ax - b)$, so the stationary points satisfy

$$A^T C A\, x \;=\; A^T C b.$$

Since $C \succ 0$ and A has full column rank, $A^T C A$ is symmetric positive definite and the equation has a unique solution, which is therefore the unique minimizer of $\|Ax - b\|_C$.

For a formulation analogous to the unweighted case, introduce the Cholesky factor $C^{1/2}$ and the auxiliary variable $r = C^{1/2}(b - Ax)$. Minimizing $\|Ax - b\|_C$ is equivalent to minimizing $\|r\|_2$ subject to the linear constraint $r + C^{1/2}A\,x = C^{1/2}b$. The KKT conditions for this problem are encoded by the symmetric block system

$$\begin{bmatrix} I & C^{1/2}A \\ A^T C^{1/2} & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} C^{1/2}b \\ 0 \end{bmatrix}.$$

Indeed, the first block row enforces $r = C^{1/2}(b - Ax)$, and the second gives $A^T C^{1/2}r = 0$, which is exactly $A^T C(Ax - b) = 0$, i.e., the weighted normal equations above. Conversely, if x satisfies $A^T C Ax = A^T C b$ and $r = C^{1/2}(b - Ax)$, then the block system holds. Equivalently, with $\widetilde{A} = C^{1/2}A$ and $\widetilde{b} = C^{1/2}b$, this is the unweighted formulation

$$\begin{bmatrix} I & \widetilde{A} \\ \widetilde{A}^T & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} \widetilde{b} \\ 0 \end{bmatrix}.$$

In the special case of diagonal weights $D = \mathrm{diag}(d_i) > 0$, one has $C = D^2$ and $C^{1/2} = D$, so this reduces to minimizing $\|D(Ax - b)\|_2$ with the same block structure. $\qquad\square$

Question 3.5

Proof. Since $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite, $\langle u, v \rangle_A := u^T A v$ is an inner product on $\mathbb{R}^n$ with norm $\|u\|_A = (u^T A u)^{1/2}$. Let $\mathcal{S} \subseteq \mathbb{R}^n$ be any subspace of dimension r and pick a basis $\{\alpha_1, \ldots, \alpha_r\}$. Define $\beta_1 = \alpha_1 / \|\alpha_1\|_A$. For $i = 2, \ldots, r$, set

$$w_i = \alpha_i - \sum_{j=1}^{i-1} \langle \alpha_i, \beta_j \rangle_A \, \beta_j, \qquad \beta_i = \frac{w_i}{\|w_i\|_A}.$$

The denominators are nonzero because if $w_i = 0$ then α_i lies in $\text{span}\{\alpha_1, \ldots, \alpha_{i-1}\}$, which contradicts linear independence. For $i > j$,

$$\langle \beta_i, \beta_j \rangle_A = \frac{1}{\|w_i\|_A} \left\langle \alpha_i - \sum_{k=1}^{i-1} \langle \alpha_i, \beta_k \rangle_A \, \beta_k, \ \beta_j \right\rangle_A = \frac{1}{\|w_i\|_A} \Big(\langle \alpha_i, \beta_j \rangle_A - \langle \alpha_i, \beta_j \rangle_A \Big) = 0,$$

and $\langle \beta_i, \beta_i \rangle_A = 1$ by construction. Thus $\{\beta_1, \ldots, \beta_r\}$ is A-orthonormal. Moreover each β_i lies in $\text{span}\{\alpha_1, \ldots, \alpha_i\}$ and the transformation from $(\alpha_1, \ldots, \alpha_r)$ to $(\beta_1, \ldots, \beta_r)$ is by a unit upper–triangular change of basis with nonzero diagonal entries, hence $\{\beta_1, \ldots, \beta_r\}$ spans $\mathcal{S}$. Therefore every subspace admits an A-orthonormal basis. Equivalently, if $U = [\beta_1 \ \cdots \ \beta_r] \in \mathbb{R}^{n \times r}$, then $U^T A U = I_r$. $\qquad\square$

Question 3.6

Proof. Let $A = \begin{bmatrix} R \\ S \end{bmatrix} \in \mathbb{R}^{(n+m)\times n}$ with $R \in \mathbb{R}^{n\times n}$ upper triangular and $S \in \mathbb{R}^{m\times n}$ dense. We construct a left orthogonal reduction that annihilates the entries of S below the diagonal without disturbing the zeros already present in R. For $i = 1, \ldots, n$ define

$$x_i = \begin{bmatrix} R_{ii} \\ S_{:,i} \end{bmatrix} \in \mathbb{R}^{m+1}.$$

Form the Householder reflector $P_i = I - 2\frac{v_i v_i^T}{v_i^T v_i}$ with $v_i = x_i \pm \|x_i\|_2 e_1$ so that $P_i x_i = \begin{bmatrix} \alpha_i \\ 0 \end{bmatrix}$ where $\alpha_i = \pm\|x_i\|_2$. Embed P_i so that it acts only on row i of R together with all rows of S, leaving the other rows of R unchanged:

$$\widehat{P}_i = \begin{bmatrix} I_{i-1} & 0 & 0 & \\ 0 & p_{11} & 0 & p_{12}^T \\ 0 & 0 & I_{n-i} & 0 \\ 0 & p_{21} & 0 & P_{22} \end{bmatrix}, \qquad P_i = \begin{bmatrix} p_{11} & p_{12}^T \\ p_{21} & P_{22} \end{bmatrix}.$$

Update $A^{(i+1)} = \widehat{P}_i A^{(i)}$ starting from $A^{(1)} = A$. In column i this gives

$$\widehat{P}_i \begin{bmatrix} R_{1:i-1,i} \\ R_{ii} \\ R_{i+1:n,i} \\ S_{:,i} \end{bmatrix} = \begin{bmatrix} R_{1:i-1,i} \\ \alpha_i \\ R_{i+1:n,i} \\ 0 \end{bmatrix},$$

so all entries of S below the ith diagonal element are zeroed while rows $i+1, \ldots, n$ of R are untouched. Since $\widehat{P}_i$ mixes only row i of R with rows of S, the strict lower part of the R block is never modified and R stays upper triangular throughout. Therefore after n steps $A^{(n+1)}$ is upper triangular:

$$A^{(n+1)} = \widehat{P}_n \cdots \widehat{P}_1 A = \begin{bmatrix} \widetilde{R} \\ 0 \end{bmatrix}, \qquad \widetilde{R} \text{ upper triangular.}$$

The cost of step i is dominated by applying P_i in compact form to the trailing submatrix consisting of row i and the m rows of S for columns $i, \ldots, n$. Using $A \leftarrow A - 2u(u^T A)$ with u the Householder vector of length $m + 1$, this requires about $2(m + 1)(n - i + 1)$ flops. Summing over i gives approximately $(m+1)n(n+1)$ flops, which is $O(mn^2)$ and strictly less than applying the standard Householder QR (Algorithm 3.2) to the full $(m+n) \times n$ matrix, which costs $O((m+n)n^2)$ and creates fill in the lower triangular part of the R block. Hence the described procedure reduces A to upper triangular form, preserves the zeros already present in R, and uses fewer operations than the unstructured algorithm. $\qquad\square$

Question 3.7

Proof. Let $A = R + uv^T \in \mathbb{R}^{n \times n}$ with R upper triangular and $u, v \in \mathbb{R}^n$. If $u = 0$ or $v = 0$ then $A = R$ and the QR factorization is trivial. Assume $u \neq 0$ and $v \neq 0$. The idea is to use left Givens rotations so that the rank–one term affects only the last row, and then "chase" a single bulge to the right until the matrix is again upper triangular.

First, by possibly applying a single row swap between row k and row n where k is the largest index with $u_k \neq 0$ (an orthogonal operation), we may assume $u_n \neq 0$. Construct $n - 1$ Givens rotations $G_1, \ldots, G_{n-1}$ acting on the pairs of rows $(1, n), (2, n), \ldots, (n-1, n)$ so that

$$G u = \|u\|_2 \, e_n, \qquad G := G_{n-1} \cdots G_1.$$

Apply G to A from the left:

$$A_1 := GA = GR + (Gu)v^T = \widetilde{R} + \alpha \, e_n v^T, \qquad \alpha = \|u\|_2,$$

where $\widetilde{R} := GR$. At this point A_1 is upper triangular except possibly in its last row, because the only contribution below the diagonal comes from the row vector $e_n v^T$.

Next, remove the entries to the left of the diagonal in the last row by a rightward bulge chase. For $j = 1, 2, \ldots, n - 1$, form a Givens rotation H_j acting on rows (j, n) of the current matrix so that the (n, j) entry is annihilated. Premultiplying by H_j affects only rows j and n; before each step the matrix is upper triangular except possibly in the last row, hence H_j creates at most one new subdiagonal element and places it in column $j + 1$. The next rotation eliminates that element and moves the bulge one column to the right. After the final step the matrix

$$R^{\text{new}} := H_{n-1} \cdots H_1 A_1$$

is upper triangular. The accumulated orthogonal factor is

$$Q^T = H_{n-1} \cdots H_1 G, \qquad \text{so} \qquad A = Q R^{\text{new}}.$$

Costs are $O(n^2)$. Each G_i mixes two rows of an upper triangular matrix and touches only the trailing part of those rows, which costs $O(n-i+1)$ flops; the total is $\sum_{i=1}^{n-1} O(n-i+1) = O(n^2)$. Each H_j also mixes two rows and touches only the trailing submatrix in columns $j, \ldots, n$, giving $\sum_{j=1}^{n-1} O(n - j + 1) = O(n^2)$. The overall work is therefore $O(n^2)$, which is asymptotically less than the $O(n^3)$ cost of applying a generic QR algorithm (Algorithm 3.2) to A. This produces the desired QR decomposition using only Givens rotations and exploits the rank–one structure of $A = R + uv^T$. $\square$

Question 3.8

Proof. No, P need not (and for $n \geq 2$ cannot) equal Q. Let $x \neq 0$ and let P be the Householder reflector that maps x to $\pm \|x\|_2 e_1$, so $P = I - 2uu^T$ with u a unit vector; every such Householder has $\det(P) = -1$. Each Givens rotation $G_{i,j}(c, s)$ is orthogonal with $\det(G_{i,j}) = 1$, hence any product $Q = G_{1,2} \cdots G_{n-1,n}$ satisfies $\det(Q) = 1$. Since two matrices with different determinants cannot be equal, for $n \geq 2$ we must have $P \neq Q$ even though both may send x to $\pm \|x\|_2 e_1$.

For a concrete counterexample in $\mathbb{R}^2$, take $x = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$, $\|x\|_2 = 5$. The Householder with $u = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}$ is

$$P = I - 2uu^T = \frac{1}{5} \begin{bmatrix} -3 & -4 \\ -4 & 3 \end{bmatrix}, \qquad Px = \begin{bmatrix} -5 \\ 0 \end{bmatrix} = -\|x\|_2 e_1,$$

and the Givens rotation

$$Q = \begin{bmatrix} -\frac{3}{5} & -\frac{4}{5} \\ \frac{4}{5} & -\frac{3}{5} \end{bmatrix}$$

also satisfies $Qx = \begin{bmatrix} -5 \\ 0 \end{bmatrix}$, but $\det(P) = -1$ while $\det(Q) = 1$, so $P \neq Q$. (The only degenerate case where equality can occur is $n = 1$, where $Q = I$ and $P = \pm I$.) □

Question 3.9

1. *Proof.* Assume $A \in \mathbb{R}^{m \times n}$ has full column rank n and let its thin SVD be $A = U\Sigma V^T$ with $U^T U = I_n$, $V^T V = I_n$, and $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ with $\sigma_i > 0$. Then

$$A^T A = V\Sigma^2 V^T \implies (A^T A)^{-1} = V\Sigma^{-2}V^T,$$

   which is the SVD of $(A^T A)^{-1}$ since it is symmetric positive definite with left and right singular vectors equal to V and singular values σ_i^{-2}. □

2. *Proof.* Using $A^T = V\Sigma U^T$,

$$(A^T A)^{-1} A^T = V\Sigma^{-2}V^T V\Sigma U^T = V\Sigma^{-1}U^T.$$

   Thus an SVD is $V\,\Sigma^{-1}\,U^T$ with singular values σ_i^{-1}, left singular vectors V, and right singular vectors U. □

3. *Proof.*
$$A(A^T A)^{-1} = U\Sigma V^T V\Sigma^{-2}V^T = U\Sigma^{-1}V^T.$$

   Hence an SVD is $U\,\Sigma^{-1}\,V^T$ with singular values σ_i^{-1}, left singular vectors U, and right singular vectors V. □

4. *Proof.*
$$A(A^T A)^{-1} A^T = U\Sigma V^T V\Sigma^{-2}V^T V\Sigma U^T = U I_n U^T = UU^T.$$

   This is the orthogonal projector onto $\mathrm{range}(A)$. Completing U to an orthogonal basis $\widehat{U} = [\,U \;\; U_\perp\,] \in \mathbb{R}^{m \times m}$, an SVD is

$$\widehat{U} \begin{bmatrix} I_n & 0 \\ 0 & 0 \end{bmatrix} \widehat{U}^T,$$

   so the singular values are 1 (repeated n times) and 0 (repeated $m - n$ times), with left and right singular vectors both equal to $\widehat{U}$. □

Question 3.10

Disproof. The statement is false for the spectral norm. I will give a concrete family of counterexamples and explain why a whole continuum of best rank–k approximants exists.

Let

$$A = \operatorname{diag}(5, 3, 1) \in \mathbb{R}^{3 \times 3}, \qquad k = 2.$$

The singular values of A are $(\sigma_1, \sigma_2, \sigma_3) = (5, 3, 1)$, so $\sigma_2 > \sigma_3$. The truncated SVD is

$$A_2 = \operatorname{diag}(5, 3, 0).$$

For any $\varepsilon \in [0, 1]$ define the rank–2 matrix

$$B_\varepsilon = \operatorname{diag}(5 - \varepsilon,\ 3,\ 0).$$

Then

$$A - B_\varepsilon = \operatorname{diag}(\varepsilon,\ 0,\ 1).$$

Because this difference is diagonal, its spectral norm equals the largest absolute diagonal entry:

$$\|A - B_\varepsilon\|_2 = \max\{\varepsilon, 1\} = 1 = \sigma_3.$$

By the Eckart–Young–Mirsky theorem, the minimum possible spectral–norm error among all rank–2 matrices is exactly σ_3. Hence every B_ε with $\varepsilon \in [0, 1]$ is a best rank–2 approximation of A. Since $B_\varepsilon \neq A_2$ for every $\varepsilon \in (0, 1]$, the best rank–k approximation is not unique even though there is a strict gap $\sigma_k > \sigma_{k+1}$.

This phenomenon is not special to the numbers above. Write the SVD as

$$A = U \operatorname{diag}(\sigma_1, \ldots, \sigma_n) V^T$$

with strictly decreasing singular values and fix $k = n - 1$. For any $t \in [0, \sigma_n]$ set

$$\widetilde{B}_t = U \operatorname{diag}(\sigma_1 - t,\ \sigma_2, \ldots, \sigma_{n-1},\ 0)\, V^T,$$

which has rank k. In the singular basis,

$$U^T(A - \widetilde{B}_t)V = \operatorname{diag}(t, 0, \ldots, 0, \sigma_n),$$

so $\|A - \widetilde{B}_t\|_2 = \max\{t, \sigma_n\} = \sigma_n$. Therefore every $\widetilde{B}_t$ is optimal and there is a continuum of distinct best rank–k approximations. The strict gap $\sigma_k > \sigma_{k+1}$ guarantees the value of the minimal error but does not enforce uniqueness in the spectral norm, because the objective depends only on the largest singular value of the residual and there is slack to redistribute up to size σ_{k+1} within the leading singular direction while keeping rank at most k.

For contrast, under the Frobenius norm the best rank–k approximation is unique when $\sigma_k > \sigma_{k+1}$, since the Frobenius error equals the ℓ_2 norm of the vector of discarded singular values and truncation at k is the only way to remove exactly $\{\sigma_{k+1}, \ldots, \sigma_n\}$. $\square$