CMDA 3606 · MATHEMATICAL MODELING II

Problem Set 6 · Solutions

Posted 7 October 2022. Due at 11:59pm on Thursday, 13 October 2022.

Please submit your problem set by uploading to Canvas one PDF file that includes all elements of your solution. Be sure to include your Python code/Jupyter notebook(s).

Basic guidelines: Students may discuss the problems on this assignment, but each student must submit his or her individual write-up and code. (In particular, you *must write up your own individual Python code.*) Students may consult the class notes and other online resources, but *the use of solutions from previous classes is forbidden and will be regarded as a violation of the Honor Code.*

1. [30 points: 5 points each for (a),(b),(c); 4 points each for (d),(e),(f); 3 points for (g)]

   The *orthogonal projector onto* $\mathcal{R}(\mathbf{A})$ plays a crucial role in understanding least squares problems. This problem asks you to consider three different approaches for constructing this projector.

   (This problem was designed to be solved by hand, but you can use Python to check your work.)

   Consider the matrix

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 2 \\ 2 & 0 & 0 \end{bmatrix}.$$

   (a) Compute the pseudoinverse $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$.

   (b) Apply the Gram–Schmidt process to the columns of $\mathbf{A}$ and use the results to obtain the factorization $\mathbf{A} = \mathbf{QR}$. (You should specify the matrices $\mathbf{Q} \in \mathbb{R}^{4\times 3}$ and $\mathbf{R} \in \mathbb{R}^{3\times 3}$.)

   (c) Compute the reduced (economy-sized SVD), $\mathbf{A} = \mathbf{U\Sigma V}^T$. (You should specify the matrices $\mathbf{U} \in \mathbb{R}^{4\times 3}$, $\mathbf{\Sigma} \in \mathbb{R}^{3\times 3}$, and $\mathbf{V} \in \mathbb{R}^{3\times 3}$.)

   (d) Construct $\mathbf{P_A} = \mathbf{AA}^+$.

   (e) Construct $\mathbf{P_Q} = \mathbf{QQ}^T$.

   (f) Construct $\mathbf{P_U} = \mathbf{UU}^T$.

   (g) Your answers to parts (d), (e), and (f) should all be the same matrix, so let us just call it $\mathbf{P}$. Show that $\mathbf{P}$ is a projector by computing $\mathbf{P}^2$ (using the numerical values in your matrix). (You should find that $\mathbf{P}^2 = \mathbf{P}$.)

Solution.

(a) Compute $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$:

$$(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T = \begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/6 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 2 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1/2 \\ 1/2 & 1/2 & 0 & 0 \\ 1/6 & -1/6 & 1/3 & 0 \end{bmatrix}.$$

(b) The Gram–Schmidt process works out very nicely, because the three columns of $\mathbf{A}$ are already orthogonal. First step:

$$\widehat{\mathbf{q}}_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \end{bmatrix}, \qquad r_{1,1} = \|\widehat{\mathbf{q}}_1\| = 2, \qquad \mathbf{q}_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

Second step:

$$\widehat{\mathbf{q}}_2 = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} - 0 \cdot \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \qquad \begin{array}{l} r_{1,2} = \mathbf{q}_1^T \mathbf{a}_2 = 0 \\ r_{2,2} = \|\widehat{\mathbf{q}}_2\| = \sqrt{2}, \end{array} \qquad \mathbf{q}_2 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}.$$

Third step:

$$\widehat{\mathbf{q}}_3 = \begin{bmatrix} 1 \\ -1 \\ 2 \\ 0 \end{bmatrix} - 0 \cdot \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} - 0 \cdot \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}, \qquad \begin{array}{l} r_{1,3} = \mathbf{q}_1^T \mathbf{a}_3 = 0 \\ r_{2,3} = \mathbf{q}_2^T \mathbf{a}_3 = 0 \\ r_{3,3} = \|\widehat{\mathbf{q}}_3\| = \sqrt{6}, \end{array} \qquad \mathbf{q}_3 = \begin{bmatrix} 1/\sqrt{6} \\ -1/\sqrt{6} \\ 2/\sqrt{6} \\ 0 \end{bmatrix}.$$

Assemble these pieces into a QR factorization:

$$\mathbf{A} = \mathbf{QR} = \begin{bmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{6} \\ 0 & 1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 0 & 2/\sqrt{6} \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{6} \end{bmatrix}.$$

(c) Use the computed $\mathbf{A}^T\mathbf{A}$ (which is diagonal!) from part (a) to determine

$$\sigma_1 = \sqrt{6}, \qquad \mathbf{v}_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \qquad \sigma_2 = 2, \qquad \mathbf{v}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \qquad \sigma_3 = \sqrt{2}, \qquad \mathbf{v}_3 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}.$$

From these singular values and right singular vectors, we can compute

$$\mathbf{u}_1 = \frac{1}{\sigma_1}\mathbf{A}\mathbf{v}_1 = \begin{bmatrix} 1/\sqrt{6} \\ -1/\sqrt{6} \\ 2/\sqrt{6} \\ 0 \end{bmatrix}, \qquad \mathbf{u}_2 = \frac{1}{\sigma_2}\mathbf{A}\mathbf{v}_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \qquad \mathbf{u}_3 = \frac{1}{\sigma_3}\mathbf{A}\mathbf{v}_3 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}.$$

Assemble the pieces to the get reduced SVD:

$$\mathbf{A} = \mathbf{U\Sigma V}^T = \begin{bmatrix} 1/\sqrt{6} & 0 & 1/\sqrt{2} \\ -1/\sqrt{6} & 0 & 1/\sqrt{2} \\ 2/\sqrt{6} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \sqrt{6} & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

(d) Compute $\mathbf{AA}^+$:

$$\mathbf{AA}^+ = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 2 \\ 2 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 1/2 \\ 1/2 & 1/2 & 0 & 0 \\ 1/6 & -1/6 & 1/3 & 0 \end{bmatrix} = \begin{bmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

(e) Compute $\mathbf{QQ}^T$:

$$\mathbf{QQ}^T = \begin{bmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{6} \\ 0 & 1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 0 & 2/\sqrt{6} \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\ 1/\sqrt{6} & -1/\sqrt{6} & 2/\sqrt{6} & 0 \end{bmatrix} = \begin{bmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

(f) Compute $\mathbf{UU}^T$:

$$\mathbf{UU}^T = \begin{bmatrix} 1/\sqrt{6} & 0 & 1/\sqrt{2} \\ -1/\sqrt{6} & 0 & 1/\sqrt{2} \\ 2/\sqrt{6} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{6} & -1/\sqrt{6} & 2/\sqrt{6} & 0 \\ 0 & 0 & 0 & 1 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \end{bmatrix} = \begin{bmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

(g) Multiply the matrices out to confirm that

$$\begin{bmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Graders: Students do not need to show more work than just writing down the matrices, as given here. However, if they have their projector wrong and somehow still write down $\mathbf{P}^2 = \mathbf{P}$ *when that is not true, please take off points.*

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2. [39 points; 20 points for (a); 15 points each for (b); 4 points for (c)]

(a) Consider the matrix and vector

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 1 \\ 2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

(i) Compute (by hand) and write out the dyadic from of the SVD (where $r = \operatorname{rank}(\mathbf{A})$):

$$\mathbf{A} = \sum_{j=1}^{r} \sigma_j \mathbf{u}_j \mathbf{v}_j^T.$$

(ii) Compute (in the form of one 3×3 matrix) the pseudoinverse

$$\mathbf{A}^+ = \sum_{j=1}^{r} \frac{1}{\sigma_j} \mathbf{v}_j \mathbf{u}_j^T.$$

(iii) Determine a basis for the null space $\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^3 : \mathbf{Ax} = \mathbf{0}\}$ of this matrix.

(iv) Any solution $\mathbf{x}$ of the least squares problem

$$\min_{\mathbf{x} \in \mathbb{R}^3} \|\mathbf{b} - \mathbf{Ax}\|$$

must have the form $\mathbf{x} = \mathbf{A}^+\mathbf{b} + \mathbf{c}$, where $\mathbf{c}$ is in the null space of $\mathbf{A}$, $\mathbf{c} \in \mathcal{N}(\mathbf{A})$. Write down a formula for all such solutions $\mathbf{x}$ for this $\mathbf{A}$ and $\mathbf{b}$.

(v) Show that, among all the solutions identified in (iii), $\|\mathbf{x}\|$ is minimized by $\mathbf{x}_+ = \mathbf{A}^+\mathbf{b}$.

(b) Now for any ε satisfying $0 < \varepsilon < 1$, consider the modified problem

$$\mathbf{A}_\varepsilon = \begin{bmatrix} 0 & 0 & 1 \\ 2 & 0 & 0 \\ 0 & \varepsilon & 0 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

(i) Compute (by hand) the dyadic form of the SVD of $\mathbf{A}_\varepsilon$.

(ii) Write down a formula for the pseudoinverse $\mathbf{A}_\varepsilon^+$.

(iii) Assuming $0 < \varepsilon < 1$, find the vector $\mathbf{x}_\varepsilon \in \mathbb{R}^3$ that solves

$$\min_{\mathbf{x}_\varepsilon \in \mathbb{R}^3} \|\mathbf{b} - \mathbf{A}_\varepsilon \mathbf{x}_\varepsilon\|.$$

(c) Now compare your results from parts (a) and (b): Let $\mathbf{x}_+$ and $\mathbf{x}_\varepsilon$ denote the solutions from (a.v) and (b.iii).
Does $\mathbf{A}_\varepsilon^+ \to \mathbf{A}^+$ as $\varepsilon \to 0$? Does $\mathbf{x}_\varepsilon \to \mathbf{x}_+$ as $\varepsilon \to 0$?
Based on your answer to these questions: Is the minimum-norm solution to a least squares problem a *continuous function* of the entries of $\mathbf{A}$? (Think about the implications of this observation for more practical problems where $\mathbf{A}$ could be polluted by rounding errors, data noise, etc.)

Solution.

(a) (i) The dyadic form of the SVD of $\mathbf{A}$ is:

$$\mathbf{A} = \mathbf{U\Sigma V}^T = 2\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \end{bmatrix} + 1\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 \end{bmatrix}.$$

(ii) The pseudoinverse is then

$$\mathbf{A}^+ = \frac{1}{\sigma_1}\mathbf{v}_1\mathbf{u}_1^T + \frac{1}{\sigma_2}\mathbf{v}_2\mathbf{u}_2^T = \frac{1}{2}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}\begin{bmatrix} 0 & 1 & 0 \end{bmatrix} + \frac{1}{1}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1/2 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

(iii) The matrix $\mathbf{A}$ clearly has two linearly independent columns, so $r = \operatorname{rank}(\mathbf{A}) = 2$. Thus, the null space has dimension $n - r = 3 - 2 = 1$. It is easy to spot a nonzero vector in the null space, and hence a basis for the one-dimensional null space:

$$\mathcal{N}(\mathbf{A}) = \operatorname{span}\left\{\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}\right\}.$$

(iv) The solutions to $\min_{\mathbf{x}\in\mathbb{R}^3} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|$ have the form $\mathbf{A}^+\mathbf{b} + \mathbf{c}$ for $\mathbf{c} \in \mathcal{N}(\mathbf{A})$. Note that $\mathcal{N}(\mathbf{A}) = \operatorname{span}\{\mathbf{v}_3\}$ for this example, since $\operatorname{rank}(\mathbf{A}) = 2$. Thus, solutions to the least squares problem have the form

$$\mathbf{x} = \mathbf{A}^+\mathbf{b} + \mathbf{c} = \begin{bmatrix} 1/2 \\ 0 \\ 1 \end{bmatrix} + \gamma\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/2 \\ \gamma \\ 1 \end{bmatrix}.$$

(v) Note that

$$\|\mathbf{x}\|^2 = \|\mathbf{A}^+\mathbf{b} + \mathbf{c}\|^2 = \left\|\begin{bmatrix} 1/2 \\ 0 \\ 1 \end{bmatrix}\right\|^2 + \left\|\begin{bmatrix} 0 \\ \gamma \\ 0 \end{bmatrix}\right\|^2 = (1/2)^2 + \gamma^2 + (1)^2 = 5/4 + \gamma^2,$$

which is minimized when $\gamma = 0$, i.e.,

$$\mathbf{x}_+ = \mathbf{A}^+\mathbf{b} = \begin{bmatrix} 1/2 \\ 0 \\ 1 \end{bmatrix}.$$

Graders: This problem is simple enough that students might simply conclude that $\gamma = 0$ by inspection. That is acceptable for full credit.

(b) (i) The dyadic form of the SVD of $\mathbf{A}_\varepsilon$ is

$$\mathbf{A} = 2\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \end{bmatrix} + 1\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 \end{bmatrix} + \varepsilon\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\begin{bmatrix} 0 & 1 & 0 \end{bmatrix}.$$

(ii) The pseudoinverse of $\mathbf{A}_\varepsilon$ is just the inverse, since $\mathbf{A}_\varepsilon$ is full-rank for all $\varepsilon > 0$:

$$\mathbf{A}_\varepsilon^+ = \mathbf{A}_\varepsilon^{-1} = \begin{bmatrix} 0 & 1/2 & 0 \\ 0 & 0 & 1/\varepsilon \\ 1 & 0 & 0 \end{bmatrix}.$$

(iii) Since $\mathbf{A}_\varepsilon$ is invertible, the least squares problem $\min_{\mathbf{x}\in\mathbb{R}^3} \|\mathbf{b} - \mathbf{A}_\varepsilon\mathbf{x}\|$ has just one solution $\mathbf{x}_\varepsilon$:

$$\mathbf{x}_\varepsilon = \mathbf{A}_\varepsilon^{-1}\mathbf{b} = \begin{bmatrix} 1/2 \\ 1/\varepsilon \\ 1 \end{bmatrix}.$$

Since $\mathbf{x}_\varepsilon$ is the only solution to the least squares problem, it is also the norm minimizing solution.

(c) The pseudoinverse and minimum-norm least-squares solution *do not converge* as $\varepsilon \to 0$:

$$\mathbf{A}_\varepsilon^+ = \begin{bmatrix} 0 & 1/2 & 0 \\ 0 & 0 & 1/\varepsilon \\ 1 & 0 & 0 \end{bmatrix} \not\to \begin{bmatrix} 0 & 1/2 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \mathbf{A} \qquad \mathbf{x}_\varepsilon = \begin{bmatrix} 1/2 \\ 1/\varepsilon \\ 1 \end{bmatrix} \not\to \begin{bmatrix} 1/2 \\ 0 \\ 1 \end{bmatrix} = \mathbf{x}_+.$$

In fact, $\|\mathbf{x}_\varepsilon\| \to \infty$ as $\varepsilon \to 0$.

Based on this observation, we conclude that *the pseudoinverse and minimum-norm least squares solution are <u>not</u> continuous functions of the entries of* $\mathbf{A}$.

If thinking of abstract $\varepsilon > 0$ is tricky, plug in a concrete value: if $\varepsilon = 0.001$, then

$$\mathbf{A}_\varepsilon^+ = \begin{bmatrix} 0 & 1/2 & 0 \\ 0 & 0 & 1000 \\ 1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{x}_\varepsilon = \begin{bmatrix} 1/2 \\ 1000 \\ 1 \end{bmatrix}.$$

As ε gets smaller, those large entries in $\mathbf{A}^+$ and $\mathbf{x}_\varepsilon$ get even larger.

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3. [31 points; 4 points each for (a),(b),(c),(g); 5 points each for (d),(e),(f)]

Consider the matrix and vector

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & 2 \\ 2 & 0 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 1 \\ -2 \\ 0 \end{bmatrix}.$$

(This problem was designed to be solved by hand, but you can use Python to assist if you like.)

(a) Find the unique vector $\mathbf{x}_+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$ that solves

$$\min_{\mathbf{x}\in\mathbb{R}^2} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|.$$

Recall that $\mathbf{b}$ can be written in the form $\mathbf{b} = \mathbf{b}_R + \mathbf{b}_N$, where $\mathbf{b}_R \in \mathcal{R}(\mathbf{A})$ and $\mathbf{b}_N \in \mathcal{N}(\mathbf{A}^T)$, and that the least squares solution $\mathbf{x}_+$ satisfies $\mathbf{A}\mathbf{x}_+ = \mathbf{b}_R$.

(b) For the particular $\mathbf{b}$ given above, compute $\mathbf{b}_R$ and $\mathbf{b}_N$.
Hint: use $\mathbf{b}_R = \mathbf{A}\mathbf{x}_+$ *and* $\mathbf{b}_N = \mathbf{b} - \mathbf{b}_R$.

(c) Compute $\|\mathbf{b}_N\|$ (recall that $\min_{\mathbf{x}\in\mathbb{R}^2} \|\mathbf{b} - \mathbf{A}\mathbf{x}\| = \|\mathbf{b}_N\|$).

The standard least squares algorithm you solved in part (a) can be viewed as a finding the vector $\mathbf{e}$ of smallest norm so that $\mathbf{b} + \mathbf{e} \in \mathcal{R}(\mathbf{A})$. (In this case, $\mathbf{e}$ is simply $-\mathbf{b}_N$.) In data fitting applications, this set-up implicitly assumes that $\mathbf{b}$ contains all the errors in the data, and $\mathbf{A}$ is known perfectly. In cases where $\mathbf{A}$ might be polluted with error too, we could instead find the smallest $\mathbf{e}$ *and* $\mathbf{E}$ such that $\mathbf{b} + \mathbf{e} \in \mathcal{R}(\mathbf{A} + \mathbf{E})$. This is called the *Total Least Squares* (TLS) problem. We measure the size of the errors $\mathbf{E}$ and $\mathbf{e}$ simultaneously by stacking $\mathbf{E}$ and $\mathbf{e}$ together in the $m \times (n+1)$ dimensional matrix $[\mathbf{E}\ \mathbf{e}]$ and computing its norm (largest singular value), $\|[\mathbf{E}\ \mathbf{e}]\|$.

To solve the TLS problem, we seek the minimal $\|[\mathbf{E}\ \mathbf{e}]\|$ such that

$$(\mathbf{A} + \mathbf{E})\mathbf{x} = (\mathbf{b} + \mathbf{e})$$

has a solution. This equation is equivalent to

$$[\,\mathbf{A} + \mathbf{E} \quad \mathbf{b} + \mathbf{e}\,] \begin{bmatrix} \mathbf{x} \\ -1 \end{bmatrix} = \mathbf{0}.$$

So, we seek the smallest $\|[\mathbf{E}\ \mathbf{e}]\|$ for which $[\mathbf{A}+\mathbf{E}\ \ \mathbf{b}+\mathbf{e}]$ has a nontrivial null space (i.e., the null space contains more than just the zero vector). If the SVD of the $m \times (n+1)$ dimensional matrix $[\mathbf{A}\ \ \mathbf{b}]$ is given (in dyadic form) by

$$[\mathbf{A}\ \ \mathbf{b}] = \sum_{j=1}^{n+1} \sigma_j \mathbf{u}_j \mathbf{v}_j^T,$$

then the smallest change $[\mathbf{E}\ \mathbf{e}]$ that makes $[\mathbf{A} + \mathbf{E}\ \ \mathbf{b} + \mathbf{e}]$ have such a null space is given by

$$[\mathbf{E}\ \mathbf{e}] = -\sigma_{n+1}\mathbf{u}_{n+1}\mathbf{v}_{n+1}^T,$$

giving the error $\|[\mathbf{E}\ \mathbf{e}]\| = \sigma_{n+1}$.

(d) Find the singular value decomposition of $[\mathbf{A}\ \mathbf{b}]$ for the $\mathbf{A}$ and $\mathbf{b}$ given above.
(*Note: Make sure you compute the SVD of the* 3×3 *matrix* $[\mathbf{A}\ \mathbf{b}]$, *not the* 3×2 *matrix* $\mathbf{A}$.)

(e) Compute $\mathbf{E}$ and $\mathbf{e}$ together as $[\mathbf{E}\ \mathbf{e}] = -\sigma_3\mathbf{u}_3\mathbf{v}_3^T$ for this example.
Note: $\mathbf{E}$ *will be the first two columns of* $-\sigma_3\mathbf{u}_3\mathbf{v}_3^T$ *and* $\mathbf{e}$ *will be the last column.*

(f) Find the solution $\mathbf{x}$ to $(\mathbf{A} + \mathbf{E})\mathbf{x} = (\mathbf{b} + \mathbf{e})$ for this example.

(g) How does the error $\|[\mathbf{E}\ \mathbf{e}]\| = \sigma_{n+1}$ for this example compare to the error $\|\mathbf{b}_N\|$ for the standard least squares problem you computed in part (c)?

Solution.

(a) One can readily compute that

$$\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b} = \begin{bmatrix} 0 \\ -3/5 \end{bmatrix}.$$

(b) The simplest approach is to recall that $\mathbf{A}\mathbf{x} = \mathbf{b}_R$, and then use $\mathbf{b}_N = \mathbf{b} - \mathbf{b}_R$:

$$\mathbf{b}_R = \mathbf{A}\mathbf{x} = \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b} = \begin{bmatrix} -3/5 \\ -6/5 \\ 0 \end{bmatrix}, \qquad \mathbf{b}_N = \mathbf{b} - \mathbf{b}_R = \begin{bmatrix} 8/5 \\ -4/5 \\ 0 \end{bmatrix}.$$

(c) Compute $\|\mathbf{b}_N\| = 4/\sqrt{5} = 1.78885\ldots$.

(d) Start with the eigenvalue decomposition

$$[\mathbf{A}\ \mathbf{b}]^T[\mathbf{A}\ \mathbf{b}] = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 5 & -3 \\ 0 & -3 & 5 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 8 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} \end{bmatrix}^T$$

The singular values are

$$\sigma_1 = \sqrt{\lambda_1} = \sqrt{8}, \qquad \sigma_2 = \sqrt{\lambda_2} = 2, \qquad \sigma_3 = \sqrt{\lambda_3} = \sqrt{2}.$$

The right singular vectors are the eigenvectors of $[\mathbf{A}\ \mathbf{b}]^T[\mathbf{A}\ \mathbf{b}]$:

$$\mathbf{v}_1 = \begin{bmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}.$$

Compute $\mathbf{u}_j = [\mathbf{A}\ \mathbf{b}]\mathbf{v}_j/\sigma_j$ to obtain

$$\mathbf{u}_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}.$$

Putting these pieces together, we obtain the (full and reduced – they are the same) SVD:

$$[\mathbf{A}\ \mathbf{b}] = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 2 & -2 \\ 2 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \sqrt{8} & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} \end{bmatrix}^T.$$

Graders: it is fine if students instead wrote this in the dyadic form.

(e) Taking the last elements of the SVD, we compute

$$[\mathbf{E}\ \mathbf{e}] = -\sigma_3\mathbf{u}_3\mathbf{v}_3^T = -\sqrt{2}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}^T = \begin{bmatrix} 0 & -1 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

(f) We seek to solve $(\mathbf{A}+\mathbf{E})\mathbf{x} = \mathbf{b}+\mathbf{e}$, i.e.,

$$(\mathbf{A}+\mathbf{E})\mathbf{x} = \begin{bmatrix} 0 & 0 \\ 0 & 2 \\ 2 & 0 \end{bmatrix}\mathbf{x} = \begin{bmatrix} 0 \\ -2 \\ 0 \end{bmatrix} = \mathbf{b}+\mathbf{e}.$$

One can readily spot that the unique solution to this system is

$$\mathbf{x} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}.$$

(g) The error of the TLS problem is $\|[\mathbf{E}\ \mathbf{e}]\| = \sigma_3 = \sqrt{2} = 1.41421\ldots$, which is significantly smaller than the ordinary least squares error $\|\mathbf{b}_N\| = 4/\sqrt{5} = 1.78885\ldots$ from part (c).

This result makes sense: When we minimize over all $\mathbf{E}$ *and* $\mathbf{e}$*, we allow for the possibility that* $\mathbf{E} = \mathbf{0}$*, which corresponds to the conventional least squares problem. By allowing perturbations to* $\mathbf{A}$ *(i.e.,* $\mathbf{E} \neq \mathbf{0}$*) we have a chance of finding a smaller norm solution. However, we can always do at least as well as* $\|[\mathbf{0}\ \mathbf{e}]\| = \|\mathbf{e}\|$*, which was the minimal error for the standard least squares problem.*

4. [20 bonus points; 2 points for (a); 3 points each for (b),(c),(e),(f); 6 points for (d)]

   Principal Component Analysis is described in Section 6.3 of the course notes; this section will provide helpful background for this problem.

   This bonus problem invites you to explore a genetics data set using Principal Component Analysis (PCA). (This example was used by in a paper by Kundu, Nambirajan, and Drineas (2013).) The GSE10072 data from the National Institutes of Health includes 22,283 genetic probes (the variables) for 107 patients, 58 of whom have lung cancer and 49 of whom do not.

   Studying all 22,283 genes would be quite a challenge; we seek to compress the data into leading principal components, following the empirical PCA procedure described in Section 6.3.3 of the class notes. (The wine data example illustrates the kind of work you will be doing on this problem.)

   Read more about the data set here: http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE10072.

   (a) Download the file `GSE10072_trimmed.txt` from Canvas and execute the following commands to create a data matrix $\mathbf{X} \in \mathbb{R}^{107\times 22{,}283}$ from the tab-separated (hence `'\t'`) data.

   ```
   import numpy as np
   import pandas as pd
   full_data = pd.read_csv('GSE10072_trimmed.txt',sep='\t')
   data = full_data.iloc[1:,1:]
   diagnoses = full_data.iloc[0,1:]
   X = data.to_numpy().T
   d = diagnoses.to_numpy()
   ```

   Execute this code in your Jupyter notebook, and verify that the resulting matrix `X` has dimension $m \times n$ with $m = 107$ and $n = 22{,}283$.

   (b) Create the centered data matrix $\mathcal{X}$ from $\mathbf{X}$ by subtracting from the jth column its mean value; call the resulting $107 \times 22{,}283$ matrix `XX`.
   Confirm that you get `XX[0,0] = 0.366487108850467`.

   (c) Compute the reduced SVD via the commands

   ```
   U, S, Vt = np.linalg.svd(XX, full_matrices=False)
   ```

   Report the *smallest* singular value. (This value should be (nearly) zero, due to the centered data.)

   (d) Produce three plots derived from the singular values, all with the index $k = 1, \ldots, m$ on the horizontal axis.

      (i) Use `plt.semilogy` to show the singular values $\sigma_1, \ldots, \sigma_m$ of $\mathcal{X}$ (i.e., the matrix you have stored as `XX`).
      Use `plt.ylim` to adjust the vertical axis so it is not skewed by the zero singular value. (The range $[10^1, 10^3]$ should look good.)

      (ii) Use `plt.semilogy` to create the "scree" plot showing the eigenvalues λ_k of the sample covariance matrix $\mathcal{X}^T\mathcal{X}/(m-1)$, adjusting the vertical axis appropriately (say, $[10^0, 10^4]$).
      Important: compute these eigenvalues from the singular values σ_k of $\mathcal{X}$ via the formula $\lambda_k = \sigma_k^2/(m-1)$. *Do not (try to) form the 22,283 × 22,283 matrix* $\mathcal{X}^T\mathcal{X}$*!*
      (The eigenvalue λ_k gives the variance of the kth principal component.)

      (iii) Use `plt.plot` to plot the cumulative sum $(\sum_{j=1}^{k} \lambda_j)/(\sum_{j=1}^{m} \lambda_j)$.
      Hint: You can use the `np.cumsum` *routine to compute the cumulative sum.*

   (e) We shall investigate how the first two principal components can identify the patients with cancer. For each of the $j = 1, \ldots, 107$ patients, the value ξ_j of the variable associated with the first principal component is given by the formula:

   ξ_j = inner product of `Vt[0,:]` (the first principal component vector) with `XX[j-1,:]`.

Similarly, the value η_j of the variable for the second principal component is given by:

η_j = inner product of `Vt[1,:]` (the second principal component vector) with `XX[j-1,:]`.

Use `plt.plot` to produce a plot showing (ξ_j, η_j) as dots for $j = 1, \ldots, 107$.

(f) Recall the vector `d` you created in part (a): `d[j-1]` equals `1.0` if the jth patient has lung cancer, and `0.0` if not.

Create another version of your plot from part (e), put now color (ξ_j, η_j) in red if the patient has cancer, and in blue if not.

Do the first two principal components distinguish between the two kinds of patients?
Briefly discuss.

(Think about this; no written answer necessary: If you were a medical doctor, how could you use this information? How might you handle a patient that was diagnosed as "no cancer" but has a (ξ_j, η_j) value close to the cluster of patients that were already diagnosed with cancer?)

Solution.

(a) Students should simply execute the given code in their Jupyter notebook.

(b) Students should subtract the mean of each column from the data. Here is one way to do it; any equivalent way to accomplish the same result is fine.

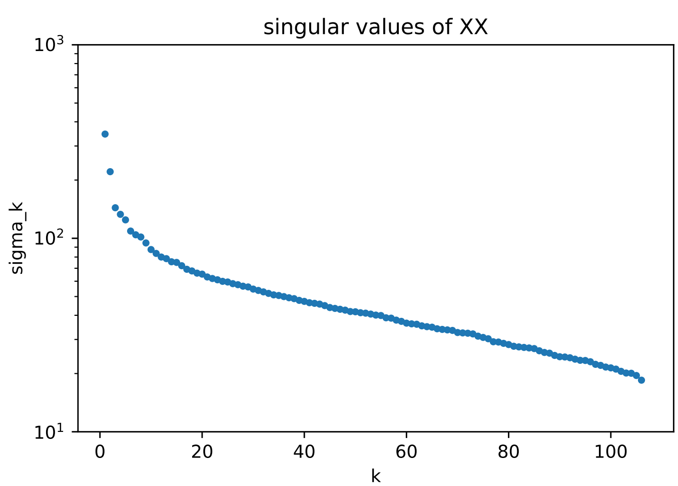
```
XX = np.zeros((m,n))
for k in range(0,n):
    XX[:,k] = X[:,k] - np.mean(X[:,k])
```

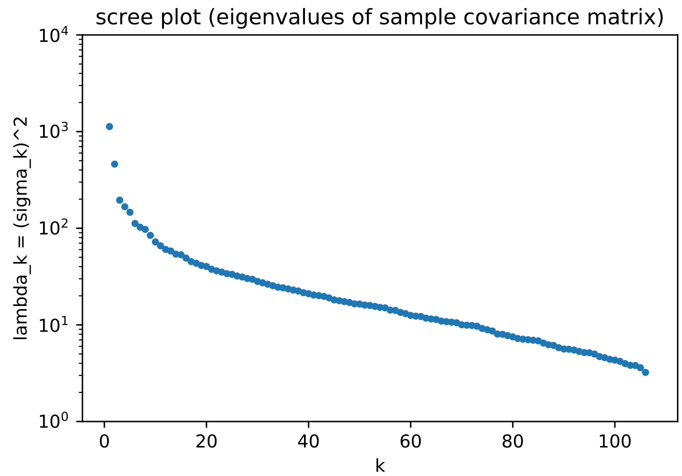
Up to minor rounding error differences, students should find that `XX[0,0] = 0.366487108850467`.

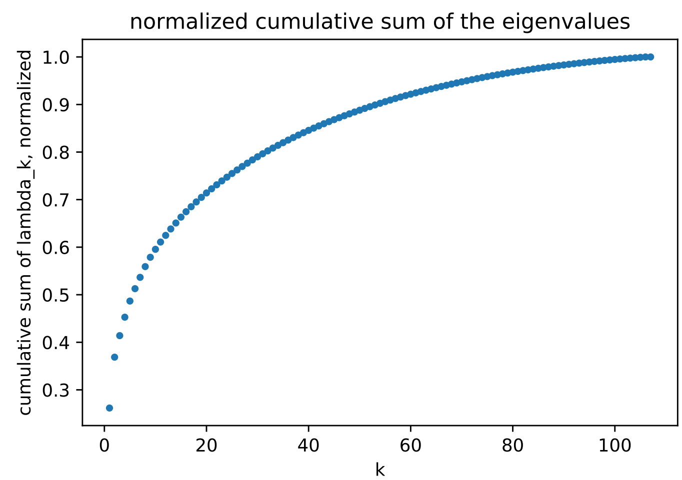
(c) The smallest singular value, as computed by my implementation, was `S[106] = 1.40029133e-12`.

Graders: students might obtain rather different values, but they should be small*, i.e., less than* 10^{-10}. *Larger values indicate that something has gone wrong, most likely when subtracting the mean from each column.*

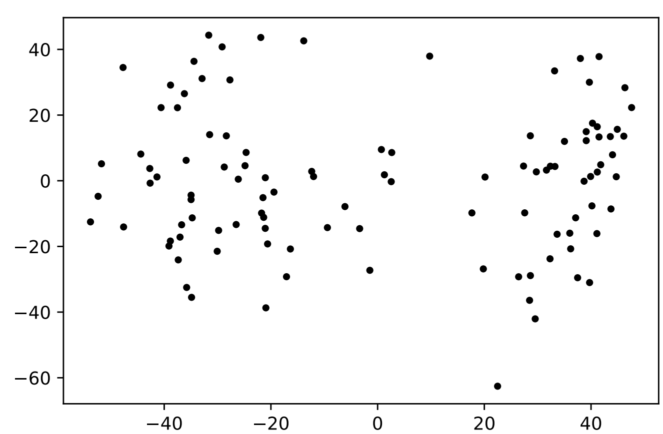
(d) The three plots requested for this question are shown below.







(e) The following plot shows the data set projected onto the first two principal components.



(f) The next plot repeats the previous one, but now color-coding the patients according to their known classification. Indeed, the first two principal components do a remarkable job of separating the patients who test positive for cancer from those who do not.

(Speaking as a mathematician and not a physician: This plot suggests that perhaps patients in the “negative” category who fall close to the boundary of these clusters should be extra vigilant for a potential occurrence of this form of cancer.)