1. Consider the 'first-order difference' matrix $A \in \mathbb{R}^{n-1 \times n}$ defined as

$$\mathbf{A} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & -1 & 1 & 0 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & -1 & 1 \end{bmatrix}$$
 (1)

We will encounter this matrix (and ones like it) later in class, and we already have tools to say a lot about the properties of this matrix. You will demonstrate that below.

(a) Does the problem $\mathbf{A}\mathbf{x} = \mathbf{b}$, where $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{b} \in \mathbb{R}^{n-1}$, have a solution? How do you know? *Hint*: it may be helpful to inspect this matrix for n = 3 or 4 and determine the answer for that case before considering the general n case.

Let's consider the case where n=4, for which **A** looks like

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

A solution does exist, since the columns of \mathbf{A} span all of \mathbb{R}^3 ; *i.e.*, $\mathcal{R}(\mathbf{A}) = \mathbb{R}^{n-1}$. We can see this by noting that any $\mathbf{b} = [b_1, b_2, b_3]^T$ can be written as $b_1 \mathbf{a}_2 + (b_2 + b_1) \mathbf{a}_3 + (b_3 + b_2 + b_1) \mathbf{a}_4$ (Try it for yourself!).

Now, we turn to the general case. It is clear from the n=4 example that for any n, $\mathcal{R}(\mathbf{A}) = \mathbb{R}^{n-1}$, as any \mathbf{b} will continue to be expressable recursively in terms of the last n-1 columns of \mathbf{A} . Thus, a solution exists for any (finite) value of n.

- (b) If there is a solution, is it unique? Why or why not? If it is not unique, what vector can be added to the solution without affecting the solution. Hint: is there a vector that gets annihilated by taking differences of its components and their neighbors?)? No, the solution is not unique because A has a nontrivial null space: multiplying A by any constant vector will result in zero. Thus, a constant vector with each entry equal to $\alpha (\in \mathbb{R})$ may be added to the solution without affecting the solution.
- 2. We derived the linear system for approximating a solution to Ax = b using the fact that if $y^* \in \mathcal{R}(A)$, then $(y^* b, r) = 0$ for any $r \in \mathcal{R}(A)$.
 - (a) Show that this is indeed true. *Hint*: any $\mathbf{w} \in \mathcal{R}(\mathbf{A})$ can be written as $\mathbf{w} = \mathbf{y}^* + \beta \mathbf{r}$ for some $\beta \in \mathbb{R}$ and $\mathbf{r} \in \mathcal{R}(\mathbf{A})$. Use this in conjunction with the fact that $||\mathbf{y}^* \mathbf{b}|| \le ||\mathbf{w} \mathbf{b}||$. Letting $\mathbf{w} \in \mathcal{R}(\mathbf{A})$ be written as as $\mathbf{w} = \mathbf{y}^* + \beta \mathbf{r}$, the inequality becomes $||\mathbf{y}^* \mathbf{b}|| \le ||(\mathbf{y}^* + \beta \mathbf{r}) \mathbf{b}||$. Writing the norms in terms of the inner product, we get

$$(y^* - b, y^* - b) \le (y^* + \beta r - b, y^* + \beta r - b,)$$
 (3)

$$= ((\boldsymbol{y}^* - \boldsymbol{b}) + \beta \boldsymbol{r}, (\boldsymbol{y}^* - \boldsymbol{b}) + \beta \boldsymbol{r},) \tag{4}$$

$$= (y^* - b, y^* - b) + 2\beta(r, (y^* - b)) + \beta^2(r, r)$$
 (5)

Subtracting $(y^* - b, y^* - b)$ from both sides of the equation gives

$$2\beta(\mathbf{r}, (\mathbf{y}^* - b)) + \beta^2(\mathbf{r}, \mathbf{r}) \ge 0 \tag{6}$$

The second term always satisfies the inequality, so the only way the inequality holds for any \boldsymbol{w} (i.e., for any β and \boldsymbol{r}) is if $(\boldsymbol{r}, (\boldsymbol{y}^* - b)) = 0$.

(b) Consider the matrix $\hat{A} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$. Determine the best approximation to the problem Ax = b onto $\mathcal{R}(A)$ for $b = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, and demonstrate the this solution indeed satisfies the required orthogonality relation.

A basis for $\mathcal{R}(\hat{A})$ is $\mathbf{v}_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$. We look for the optimal $\mathbf{y}^* = \alpha_1 \mathbf{v}_1$ that best approximates $\mathbf{A}\mathbf{x} = \mathbf{b}$. To solve for α_1 we use the orthogonality relation we just derived:

$$\alpha_1(\boldsymbol{v}_1, \boldsymbol{v}_1) = (\boldsymbol{v}_1, \boldsymbol{b}) \tag{7}$$

$$\implies \qquad \alpha_1 = \frac{(\boldsymbol{v}_1, \boldsymbol{b})}{(\boldsymbol{v}_1, \boldsymbol{v}_1)} = \frac{3}{5} \tag{8}$$

The best approximation is then $y^* = 3/5 \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

As we demonstrated must be true in a), we see that

$$(\boldsymbol{y}^* - \boldsymbol{b}, \eta \boldsymbol{v}_1) = \begin{pmatrix} \frac{3}{5} \begin{bmatrix} 1\\2 \end{bmatrix} - \begin{bmatrix} 1\\1 \end{bmatrix}, \eta \begin{bmatrix} 1\\2 \end{bmatrix} \end{pmatrix}$$
(9)

$$= \left(\begin{bmatrix} -2/5 \\ 1/5 \end{bmatrix}, \eta \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right) \tag{10}$$

$$= -2\eta/5 + 2\eta/5 \tag{11}$$

$$=0 \quad \text{for any } \eta \in \mathbb{R}$$
 (12)

3. An alien spacecraft has crash landed on Earth and biologists were able to measure concentrations of an unknown chemical as a function of radius from the crash-sight. The values of concentration (y) and radius (x) are as follows:

$$\boldsymbol{x} = \begin{bmatrix} 0.02 \\ 0.10 \\ 0.32 \\ 0.66 \\ 0.94 \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} 1.93 \\ 2.60 \\ 3.03 \\ 3.97 \\ 4.89 \end{bmatrix}$$
(13)

The biologists are turning to you to ask you to determine a line that best fits this data. That is, they want a best approximation to the problem

$$y = ax + be (14)$$

where $a,b \in \mathbb{R}$ are the constants to be solved for and $e = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$. Can you help Planet Earth?!

Once you have solved for a, b, provide a plot that includes both the raw data (with circles or some comparable marker) as well as the best fit line through the data.

We are looking for a y which is a linear combination of x and e; *i.e.*, it is in the span of $\{x, e\}$. One way to see that we want our solution to be in the span of $\{x, e\}$ is to recast the problem as

$$\begin{bmatrix} | & | \\ \boldsymbol{x} & \boldsymbol{e} \\ | & | \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} | \\ \boldsymbol{y} \\ | \end{bmatrix}$$
 (15)

We note that \boldsymbol{x} and \boldsymbol{e} are linearly independent and therefore form a basis for $\{\boldsymbol{x},\boldsymbol{e}\}$. So we can write our minimizer \boldsymbol{y}^* as $\boldsymbol{y}^* = \alpha \boldsymbol{x} + \beta \boldsymbol{e}$, where α and β are as yet unknown and are solved for from the linear system resulting from the orthogonality condition:

$$\begin{bmatrix} (\boldsymbol{x}, \boldsymbol{x}) & (\boldsymbol{x}, \boldsymbol{e}) \\ (\boldsymbol{e}, \boldsymbol{x}) & (\boldsymbol{e}, \boldsymbol{e}) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} (\boldsymbol{x}, \boldsymbol{y}) \\ (\boldsymbol{e}, \boldsymbol{y}) \end{bmatrix}$$
(16)

Plugging everything into Matlab (see code at the end of the problem), we get that $\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 2.977 \\ 2.0691 \end{bmatrix}$. The plots of the raw data and the best-fit line are provided in figure 1.

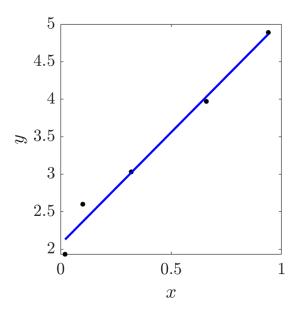


Figure 1: A plot of the raw data (black markers) and the best-fit solution (blue line).

```
%raw data
x = [0.02; 0.1; 0.32; 0.66; 0.94];
y = [1.93; 2.60; 3.03; 3.97; 4.89];
e = ones( size( x ) );
%plot raw data and hold on
plot(x, y, 'k.', 'markersize', 16), hold on
%set up and solve approximation problem:
A = [x'*x x'*e; x'*e e'*e];
b = [x'*y; e'*y];
soln = A \ b %always use \ instead of inv()
plot(x, soln(1)*x + soln(2)*e, 'b-', 'linewidth', 2)
%make plot pretty
xlabel( '$x$', 'fontsize', 16, 'interpreter', 'latex' )
ylabel( '$y$', 'fontsize', 16, 'interpreter', 'latex' )
set( gca, 'fontsize', 16, 'ticklabelinterpreter', 'latex' )
%format and save
set(gcf, 'PaperPositionMode', 'manual')
set(gcf, 'Color', [1 1 1])
set(gca, 'Color', [1 1 1])
set(gcf, 'PaperUnits', 'centimeters')
set(gcf, 'PaperSize', [10 10])
set(gcf, 'Units', 'centimeters')
set(gcf, 'Position', [0 0 10 10])
set(gcf, 'PaperPosition', [0 0 10 10])
dirsv = '~/Desktop/';
svnm = 'best_fit';
print( '-dpng', [dirsv, svnm], '-r200')
```

4. We showed in class that when the problem $\mathbf{A}\mathbf{x} = \mathbf{b}$ (with $\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{x} \in \mathbb{R}^n, \mathbf{b} \in \mathbb{R}^m$) does not have a solution, then we can approximate this solution using a basis $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}$ for $\mathcal{R}(\mathbf{A})$. Re-derive these equations assuming that the basis is orthogonal; *i.e.*, when $(\mathbf{v}_i, \mathbf{v}_j) = 0$ for $i \neq j$. What simplifications arise, and what are some benefits of these simplifications?

We write the approximation problem as

$$\min_{\boldsymbol{y} \in \mathcal{R}(\boldsymbol{A})} ||\boldsymbol{y} - \boldsymbol{b}|| \tag{17}$$

If $\{v_1, v_2, \dots, v_k\}$ forms a basis for $\mathcal{R}(A)$ then we may write the minimizer (let's call it u) as $u = \sum_{i=1}^k \alpha_i v_i$ for some as-yet undetermined coefficients α_i . Now we may use the fact that, as we just showed in problem 2, (u - b, r) = 0 for any $r \in \mathcal{R}(A)$. Since this holds for any $r \in \mathcal{R}(A)$, we may use choose k different r: $r = v_j$, $j = 1, \dots, k$. This leads us with k

different equations:

$$(\boldsymbol{u} - \boldsymbol{b}, \boldsymbol{v}_j) = 0, \quad j = 1, \dots, k$$
(18)

$$\implies (\boldsymbol{u}, \boldsymbol{v}_j) = (\boldsymbol{b}, \boldsymbol{v}_j), \quad j = 1, \dots, k$$
 (19)

$$\implies \left(\sum_{i=1}^{k} \alpha_i \mathbf{v}_i, \mathbf{v}_j\right) = (\mathbf{b}, \mathbf{v}_j), \quad j = 1, \dots, k$$
 (20)

$$\implies \sum_{i=1}^{k} \alpha_i(\mathbf{v}_i, \mathbf{v}_j) = (\mathbf{b}, \mathbf{v}_j), \quad j = 1, \dots, k$$
 (21)

$$\implies \alpha_j(\boldsymbol{v}_j, \boldsymbol{v}_j) = (\boldsymbol{b}, \boldsymbol{v}_j), \quad j = 1, \dots, k$$
 (22)

$$\implies \alpha_j = \frac{(\boldsymbol{b}, \boldsymbol{v}_j)}{(\boldsymbol{v}_j, \boldsymbol{v}_j)}, \quad j = 1, \dots, k$$
 (23)

This is a huge simplification—it turns a full linear system of equations into a set of scalar equations for the unknown coefficients!