

Homework 2 solutions

1. *Exercise A1.7.*

$$\begin{aligned}
 J &= \frac{1}{n} \|c_1 \mathbf{1} + c_2 a - b\|^2 \\
 &= \frac{1}{n} \|c_2(a - m_a \mathbf{1}) - (b - m_b \mathbf{1})\|^2 \\
 &= \frac{1}{n} (c_2^2 \|a - m_a \mathbf{1}\|^2 + \|b - m_b \mathbf{1}\|^2 - 2c_2(a - m_a \mathbf{1})^T(b - m_b \mathbf{1})) \\
 &= c_2^2 s_a^2 + s_b^2 - 2c_2 \rho s_a s_b \\
 &= \rho^2 s_b^2 + s_b^2 - 2\rho^2 s_b^2 \\
 &= (1 - \rho^2) s_b^2.
 \end{aligned}$$

On line 2, we use $c_1 = m_b - c_2 m_a$. On line 4, we use the definitions of s_a , s_b , and ρ .
On line 5, we use $c_2 = \rho s_b / s_a$.

2. *Exercise A1.8.*

(a) We first expand the square in the numerator of J :

$$\begin{aligned}
 J &= \frac{(c_1 \mathbf{1} + c_2 a - b)^T (c_1 \mathbf{1} + c_2 a - b)}{n(1 + c_2^2)} \\
 &= \frac{c_1^2 n + 2c_1 \mathbf{1}^T(c_2 a - b) + \|c_2 a - b\|^2}{n(1 + c_2^2)} \\
 &= \frac{c_1^2 + 2c_1(c_2 m_a - m_b) + \|c_2 a - b\|^2}{(1 + c_2^2)}.
 \end{aligned}$$

The derivative with respect to c_1 is

$$\frac{2(c_1 + c_2 m_a - m_b)}{(1 + c_2^2)}.$$

Setting this to zero gives $c_1 = m_b - c_2 m_a$. The orthogonal distance regression line passes through the point of averages (m_a, m_b) in the scatter plot: $m_b = c_1 + c_2 m_a$.

(b) The numerator in the expression for J is

$$\begin{aligned}
 &\|c_2(a - m_a \mathbf{1}) - (b - m_b \mathbf{1})\|^2 \\
 &= c_2^2 \|a - m_a \mathbf{1}\|^2 + \|b - m_b \mathbf{1}\|^2 - 2c_2(a - m_a \mathbf{1})^T(b - m_b \mathbf{1}) \\
 &= n(c_2^2 s_a^2 + s_b^2 - 2\rho c_2 s_a s_b).
 \end{aligned}$$

Setting the derivative of J with respect to c_2 to zero gives an equation

$$\frac{2s_a^2 c_2 - 2\rho s_a s_b}{1 + c_2^2} - \frac{2c_2(s_a^2 c_2^2 + s_b^2 - 2\rho s_a s_b c_2)}{(1 + c_2^2)^2} = 0.$$

After simplifications this reduces to the quadratic equation in the problem statement.

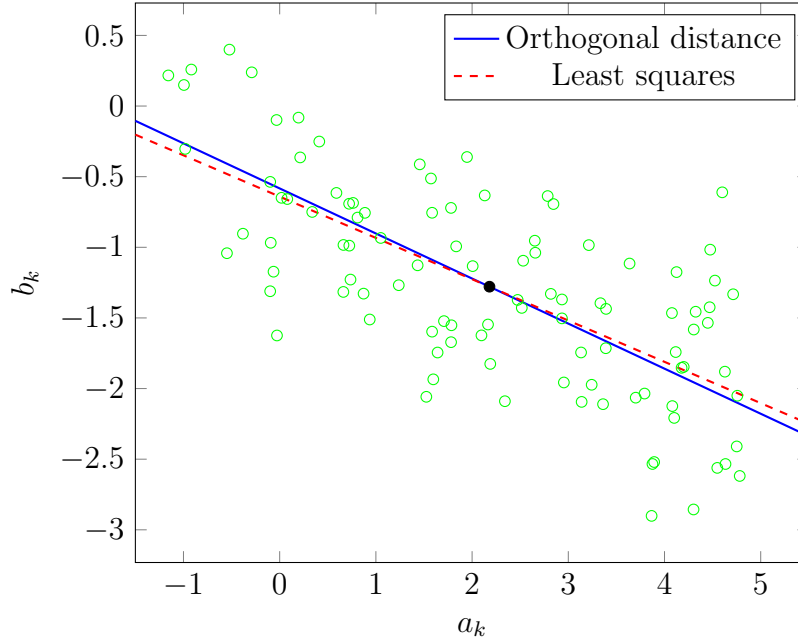
To see that the root with the same sign as ρ is the correct one, note that J approaches a limit s_a^2 as $c_2 \rightarrow \infty$ and $c_2 \rightarrow -\infty$. Also the derivative has two roots, one positive and one negative. One of these roots must correspond to a maximum of J and the other to a minimum. If $\rho > 0$ the derivative of J at $c_2 = 0$ is negative. Therefore the positive root is a minimum. If $\rho < 0$ the derivative of J at $c_2 = 0$ is positive, and the negative root is a minimum.

This choice also makes intuitive sense, because we expect the optimal slope to have the same sign as ρ , as it does for the (least squares) regression line (see, for example, the scatter plots on page 40 of lecture 2).

(c) The table gives the two solutions.

	c_1	c_2
Least squares	-0.64117	-0.29243
Orthogonal distance	-0.58323	-0.31900

The solid line in the figure is the orthogonal distance regression fit. The dashed line is the least squares fit. The black dot indicates the point of averages (m_a, m_b) .



3. *Exercise A2.4.* Define $B = I + A$. This is a nonnegative matrix, with the same off-diagonal elements as A and positive elements on the diagonal.

The diagonal elements of B^2 are

$$(B^2)_{ii} = \sum_{k=1}^n B_{ik}B_{ki} = B_{ii}^2 + \sum_{k \neq i} B_{ik}B_{ki}.$$

This is always positive because B_{ii} is positive.

Consider the off-diagonal element $(B^2)_{ij}$ with $i \neq j$:

$$(B^2)_{ij} = B_{ii}B_{ij} + B_{ij}B_{jj} + \sum_{\substack{k \neq i \\ k \neq j}} B_{ik}B_{kj}.$$

Since B_{ii} and B_{jj} are positive, the first two terms are nonzero if and only if $B_{ij} > 0$, *i.e.*, there exists an arc $j \rightarrow i$. The sum on the right-hand side is positive if and only if there is at least one k with $B_{ik} > 0$ and $B_{kj} > 0$, *i.e.*, there exists a directed path $j \rightarrow k \rightarrow i$ of length two. We can summarize this by saying that $(B^2)_{ij}$ is positive if and only if there is a directed path of length two or less from vertex j to vertex i .

In a similar way, one proves that the diagonal elements of B^m are positive, and that an off-diagonal element $(B^m)_{ij}$ is positive if and only if there is a directed path of length m or less from vertex j to vertex i . This can be seen by induction. Suppose the statement is correct for B^{m-1} . The diagonal element $(B^m)_{ii}$ is

$$(B^m)_{ii} = (B^{m-1})_{ii}B_{ii} + \sum_{k \neq i} (B^{m-1})_{ik}B_{ki}.$$

This is always positive because $B_{ii} > 0$ and $(B^{m-1})_{ii} > 0$. Consider $i \neq j$. The element $(B^m)_{ij}$ is

$$(B^m)_{ij} = \sum_{k=1}^n (B^{m-1})_{ik}B_{kj} = (B^{m-1})_{ii}B_{ij} + (B^{m-1})_{ij}B_{jj} + \sum_{\substack{k \neq i \\ k \neq j}} (B^{m-1})_{ik}B_{kj}.$$

The first term is positive if there is an arc $j \rightarrow i$. The second term is positive if $(B^m)_{ij} > 0$, *i.e.*, there is a directed path of length $m - 1$ or less from j to i . The term $(B^{m-1})_{ik}B_{kj}$ in the sum is positive if there is an arc $j \rightarrow k$ and a directed path of length $m - 1$ or less from k to i . Together, these form a directed path of length m or less from j to i that starts with the arc $j \rightarrow i$. All these cases can be summarized by saying that $(B^m)_{ij} > 0$ if and only if there is a directed path of length m or less from j to i .

In a strongly connected graph, there is a directed path from every vertex to every other vertex. Since there are only n vertices, it is sufficient to consider paths of length $n - 1$ or less. In a strongly connected graph there is a path of length $n - 1$ or less from every vertex to every other vertex. Equivalently, $B^{n-1} = (I + A)^{n-1}$ has positive elements.

4. *Exercise A2.8.* We first compute the n matrix-vector products

$$z_1 = Bx_1, \quad z_2 = Bx_2, \quad \dots, \quad z_n = Bx_n.$$

This takes $n(2n^2) = 2n^3$ flops. We then compute

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} A_{11}z_1 + A_{12}z_2 + \dots + A_{1n}z_n \\ \vdots \\ A_{n1}z_1 + A_{n2}z_2 + \dots + A_{nn}z_n \end{bmatrix},$$

where we partitioned y in subvectors y_1, \dots, y_n of size n . For each y_k this involves n scalar-vector products $A_{ki}z_i$ and $n - 1$ vector additions of size n . This takes $2n^2$ operations, so the total for computing y_1, \dots, y_n is $2n^3$.

The total flop count is $4n^3$, an order less than for a general product of this dimension (which takes $2(n^2)^2 = 2n^4$ flops).

To derive the complexity, we can also note that

$$\begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix} = B \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix} A^T,$$

so y can be computed using two matrix-matrix products of size $n \times n$, *i.e.*, in $4n^3$ flops.

5. (a) If we compute the product $A_i A_{i+1} \dots A_j$ as

$$A_i A_{i+1} \dots A_j = (A_i \dots A_k)(A_{k+1} \dots A_j),$$

the number of flops is

$$c_{ik} + c_{k+1,j} + 2n_{i-1}n_k n_j.$$

The first term is the cost of computing $A_i \dots A_k$, the second term is the cost of computing $A_{k+1} \dots A_j$, and the third term is for the product of these two matrices, which have dimensions $n_{i-1} \times n_k$ and $n_k \times n_j$, respectively. The best choice of k is the one that minimizes $c_{ik} + c_{k+1,j} + 2n_{i-1}n_k n_j$.

(b) We find

$$\begin{array}{llll} c_{11} = 0 & c_{12} = 10^{10} & c_{13} = 1.2 \cdot 10^{10} & c_{14} = 1.21 \cdot 10^9 \\ & c_{22} = 0 & c_{23} = 10^{11} & c_{24} = 1.20 \cdot 10^9 \\ & & c_{33} = 0 & c_{34} = 2 \cdot 10^8 \\ & & & c_{44} = 0. \end{array}$$

So the flop counts for $A_1 A_2 A_3 A_4$ and $A_1 A_2 A_3$ are

$$c_{14} = 1.21 \cdot 10^9 \text{ flops}, \quad c_{13} = 1.20 \cdot 10^{10} \text{ flops},$$

respectively. We note that $A_1 A_2 A_3 A_4$ is cheaper to compute than $A_1 A_2 A_3$. This is explained by the fact that the optimal order is different. For the first three matrices, the optimal order is $(A_1 A_2) A_3$. For the four matrices, the optimal order is $A_1 (A_2 (A_3 A_4))$ and this does not require computing $A_1 A_2 A_3$.