DM561 — Linear Algebra with Applications

Sheet 6, Fall 2020

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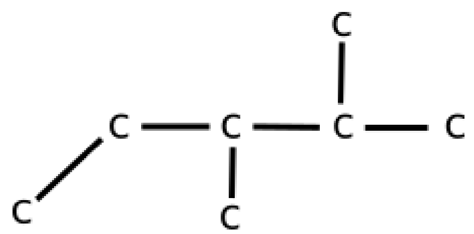
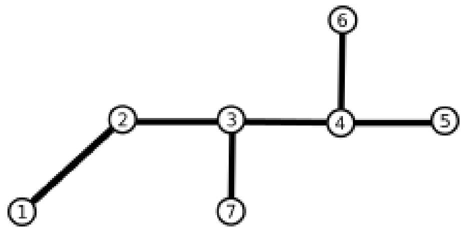
Exercise 1

(1) Extract the carbon backbone



Draw in more usually way for a Computer Scientist:



Infer edge-weight matrix

$$\begin{bmatrix} 0 & 1 & \infty & \infty & \infty & \infty & \infty \\ 1 & 0 & 1 & \infty & \infty & \infty & \infty \\ \infty & 1 & 0 & 1 & \infty & \infty & 1 \\ \infty & \infty & 1 & 0 & 1 & 1 & \infty \\ \infty & \infty & \infty & 1 & 0 & \infty & \infty \\ \infty & \infty & \infty & 1 & \infty & 0 & \infty \\ \infty & \infty & 1 & \infty & \infty & \infty & 0 \end{bmatrix}$$

(2) Compute distance matrix (to speed up we use repeated squaring)

$$W^2 = W \odot W = \begin{bmatrix} 0 & 1 & 2 & \infty & \infty & \infty & \infty \\ 1 & 0 & 1 & 2 & \infty & \infty & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1 \\ \infty & 2 & 1 & 0 & 1 & 1 & 2 \\ \infty & \infty & 2 & 1 & 0 & 2 & \infty \\ \infty & \infty & 2 & 1 & 2 & 0 & \infty \\ \infty & 2 & 1 & 2 & \infty & \infty & 0 \end{bmatrix}$$

$$W^4 = W^2 \odot W^2 = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 1 & 2 \\ 4 & 3 & 2 & 1 & 0 & 2 & 3 \\ 4 & 3 & 2 & 1 & 2 & 0 & 3 \\ 3 & 2 & 1 & 2 & 3 & 3 & 0 \end{bmatrix}$$

We could continue, but the longest path in the graph is of length 4 so $W^4 = W^5 = \dots$. Thus, $D = W^4$.

(3) The wiener index is

$$W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} D_{ij} = 46$$

(the sum of all entries in the upper triangle of D)

(4) Looking at the upper (or lower) triangular part of the distance matrix and count the occurrences of 3, we find the number of shortest paths of length 3.

There are 6 shortest paths of length 3.

(5) The value of p_0 is

$$p_0 = n - 3 = 4$$

and the value of w_0 is

$$w_0 = \frac{1}{6}(n+1)n(n-1) = \frac{1}{6}\cdot 8\cdot 7\cdot 6 = 56$$

where $n = 7$ (number of carbon atoms/vertices).

(6) The value of t_0 is

$$t_0 = 745.42 \cdot \log_{10}(n + 4.4) - 689.4 = 98.44$$

The value of t_B (estimated boiling point) is

$$t_B = t_0 - \left(\frac{98}{n^2}\cdot (w_0 - W(G)) + 5.5\cdot (p_0 - p)\right) = 89.44°C$$

(again, $n = 7$ (number of carbon atoms/vertices))

The real boiling point is $89.7°C$ according to a wikipedia search, ie. it is fairly close to the predicted value.

(7) The worst case performance for finding the distance matrix based on repeated squaring is $O(n^3 \log n)$. Each modified matrix-matrix multiplication take $O(n^3)$ time and we perform $\log_2 n$ matrix-matrix multiplications.

(8) You could use the Floyd-Warshall algorithm (solves all-pairs shortest distance problem) with asymptotic worst case performance $O(n^3)$.

Remark: Knowledge about the Floyd-Warshall algorithm comes from DM507 which students enrolled in DM562 might not have followed yet.

Exercise 2

(1) They can be use to obtain updated coordinates when (x_1, y_1), (x_2, y_2), $\ldots$, (x_n, y_n) are represented as vectors in $\mathbb{R}^n$:

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

The update computes midpoints between connected points.

(2) Only M_3 is invertible (see [2, p. 25] or next sub-exercises)

(3) The determinants are

$$\det(M_3) = \begin{vmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = 0.25 \qquad \text{(invertible)}$$

and

$$\det(M_4) = \begin{vmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{vmatrix} = 0 \qquad \text{(not invertible)}$$

(4)
- M_3: Yes - follows from Theorem 4.8.4 [1, p. 228].
- M_4: No - follows from Theorem 4.8.4 [1, p. 228].

  Note: Since the 4^{th} column is a linear combination of the others

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

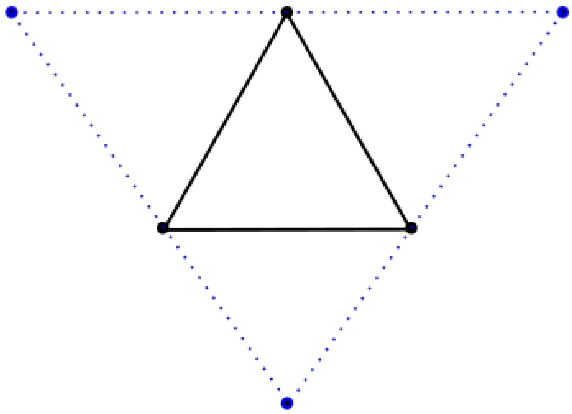
  (see Theorem 4.3.1 [1, p. 189])

(5) The proof the not written down formally but the idea is following:

- Do cofactor expansion on first column and realize that only the terms involving the first row first column and last row first column matters. When computing the determinant of the submatrix, for the term involving first row first column we are looking at a triangular matrix. Likewise, we are looking at a triangular matrix when removing the last row first column.
- Observe these sub-(triangular)-matrices always have non-zero values of the diagonal (namely, $\frac{1}{2}$ as each entry), so they determinant are non-zero and are the same for both submatrices.
- When n is even, the two terms cancel each other out given a determinant of 0 (M_n is not invertible). When n is odd, the two terms don't cancel each other out (M_n is invertible).

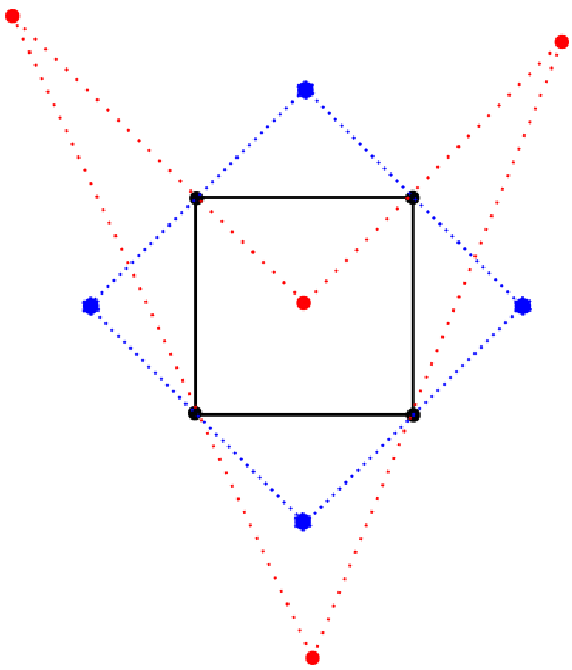
(6) Drawing an equilateral triangle with points (x_1^k, y_1^k), (x_2^k, y_2^k), and (x_3^k, y_3^k), we can find unique points (x_1^{k-1}, y_1^{k-1}), (x_2^{k-1}, y_2^{k-1}), (x_3^{k-1}, y_3^{k-1}) s.t. $x^k = M_3 \cdot x^{k-1}$ and $y^k = M_3 \cdot y^{k-1}$.

Why? Since M_3 is invertible we know there are unique solutions to $x^k = M_3 \cdot x^{k-1}$ and $y^k = M_3 \cdot y^{k-1}$, namely, $x^{k-1} = M_3^{-1} \cdot x^k$ and $y^{k-1} = M_3^{-1} \cdot y^k$. See an illustration of the situation in Figure (6).



(7) Drawing a square with points (x_1^k, y_1^k), (x_2^k, y_2^k), (x_3^k, y_3^k), and (x_4^k, y_4^k), we can find infinitely many points (x_1^{k-1}, y_1^{k-1}), (x_2^{k-1}, y_2^{k-1}), (x_3^{k-1}, y_3^{k-1}), and (x_4^{k-1}, y_4^{k-1}) s.t. $x^k = M_4 \cdot x^{k-1}$ and $y^k = M_4 \cdot y^{k-1}$.

Why? Solving the systems $x^k = M_4 \cdot x^{k-1}$ and $y^k = M_4 \cdot y^{k-1}$ can yield zero solutions, one unique solution, or infinitely many solutions for x^{k-1} and y^{k-1}. Below we show two different set of four points leading to a square when the associated vectors x^{k-1} and y^{k-1} are multiplied by M_4. Therefore, there are infinitely many solutions.



Exercise 3

(1) The average of v is

$$\frac{0 + 3 + (-1) + 11 + (-3)}{5} = 2$$

and thus $\bar{v}$ is

$$\bar{v} = \begin{pmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 2 \end{pmatrix}$$

The value of w is

$$w = v - \bar{v} = \bar{v} = \begin{pmatrix} 0 \\ 3 \\ -1 \\ 11 \\ -3 \end{pmatrix} - \begin{pmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 2 \end{pmatrix} = \begin{pmatrix} -2 \\ 1 \\ -3 \\ 9 \\ -5 \end{pmatrix}$$

Remark: The mean of w is 0. To prove that the mean of $w = v - \bar{v}$, where $\bar{v}$ is a vector where each entry is the mean of all values v_i, is 0 for an arbitrary vector $v \in \mathbb{R}^n$, do the following. Let m be the average of the entries of v. Observe the mean of the entries of w is

$$\begin{aligned} \frac{w_1 + w_2 + \cdots + w_n}{n} &= \frac{(v_1 - m) + (v_2 - m) + \cdots + (v_n - m)}{n} \\ &= \frac{(v_1 + v_2 + \cdots + v_n) - n \cdot m}{n} \\ &= \frac{(v_1 + v_2 + \cdots + v_n)}{n} - \frac{n \cdot m}{n} \\ &= m - m \\ &= 0 \end{aligned}$$

(2) Normalizing w gives

$$\frac{w}{||w||_2} = \frac{1}{\sqrt{(-2)^2 + 1^2 + (-3)^2 + 9^2 + (-5)^2}} \begin{pmatrix} -2 \\ 1 \\ -3 \\ 9 \\ -5 \end{pmatrix} = \frac{1}{\sqrt{120}} \begin{pmatrix} -2 \\ 1 \\ -3 \\ 9 \\ -5 \end{pmatrix} = \begin{pmatrix} -\frac{2}{\sqrt{120}} \\ \frac{1}{\sqrt{120}} \\ -\frac{3}{\sqrt{120}} \\ \frac{9}{\sqrt{120}} \\ -\frac{5}{\sqrt{120}} \end{pmatrix}$$

(3) The lenght of $\frac{w}{||w||_2}$ is

$$\left|\left|\frac{w}{||w||_2}\right|\right| = \sqrt{\left(-\frac{2}{\sqrt{120}}\right)^2 + \left(\frac{1}{\sqrt{120}}\right)^2 + \left(-\frac{3}{\sqrt{120}}\right)^2 + \left(\frac{9}{\sqrt{120}}\right)^2 + \left(-\frac{5}{\sqrt{120}}\right)^2} = 1$$

Exercise 4

(1) Just do it!

```
In [1]: 0.1+0.2
Out[1]: 0.30000000000000004
```

See `https://docs.python.org/3.6/tutorial/floatingpoint.html` for an explaination.

(2) (a) In all cases we except the same result mathematically, namely, that $c = a$ is true.

(b) I guess all of them.

The obvious problem with (a) is a at some point will become closer to the representation of 0. When this occurs, no matter how many times you multiply a by 2, a will always remain 0.

In (b), adding 1 after each division is introduced; thereby, the 0-problem from (a) is removed. However, at some point a will get to close to 2; thus, the second for-loop just subtracts 1 from 2 and multiplies the result by 2 obtaining 2 again.

In (c), adding 10000 after each division also removes the 0-problem from (a), however, a similar problem to (b) is that a becomes increasingly close to 20000. If a becomes 20000, then subtracting 10000 from 20000 and multiplying by 2 just gives 20000 again.

(c) In (a) the value of c should be high since it should have been exposed to a lot of division.

In (b), the value of c should also be relatively high (however less than in (a)).

In (c), the value of c should be around the same as for (b) (maybe a bit less) before creating a numerical issue.

(d) Since as observed in [2, p. 26-27], numerical issues occur in our approach to the "From Random Polygon to Ellipse" problem, and therefore we should be aware of it.

References

[1] Howard Anton and Chris Rorres. *Elementary Linear Algebra*. Springer, 11 edition, 2010.

[2] Daniel Merkle. From random polygon to ellipse. URL `https://dm561.github.io/assets/DM561-DM562-RandomPolygon.pdf`, 2020.

[3] William Stallings. *Computer Organization and Architecture: Designing for Performance*. Pearson, 10 edition, 2016.