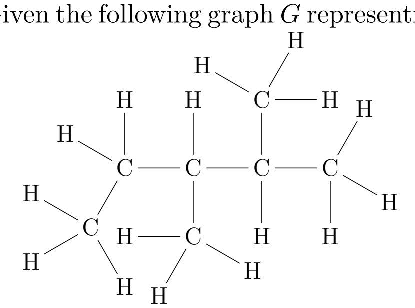
Exercise 1: (Wiener index and boiling points)
Given the following graph G representing the chemical compound 2,3-dimethylpentan:



1. Determine the edge-weight matrix of the graph of the carbon backbone.
2. Determine the distance matrix.
3. Determine the Wiener-Index.
4. Determine the number of shortest paths of length 3.
5. Determine the value p_0 and w_0 of the formula for predicting the boiling point for this compound.
6. Determine the estimated boiling points and compare it to the real boiling point.
7. What is the asymptotic worst case performance for finding the distance matrix based on repeated squaring?
8. Do you know a method that has a better asymptotic worst case performance?

Exercise 2: (From random polygon to an ellipse)

Given the matrices

$$M_3 = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$$

and

$$M_4 = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

1. How do theses matrices relate to the lecture “From Random Polygon to Ellipse”?
2. Which of both matrices is invertible?
3. Compute the determinant of M_3 and M_4.

4. Are the columns of M_3 independent? Are the columns of M_4 independent?

5. If A is a triangular matrix, i.e. $a_{ij} = 0$, whenever $i > j$ or, alternatively, whenever $i < j$, then its determinant equals the product of the diagonal entries.

   Use this fact is order to prove for all values of $k \geq 3$ if the matrix M_k is invertible or is not invertible.

6. Draw an equilateral triangle with points (x_1^k, y_1^k), (x_2^k, y_2^k), and (x_3^k, y_3^k). Assume the triangle is a result of $M_3 \cdot x^{k-1}$ and $M_3 \cdot y^{k-1}$ as presented in the lecture. Ignoring normalization, find x^{k-1} and y^{k-1}. Can you find several solutions for x^{k-1} and y^{k-1}?

7. Draw 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) . Assume the square is a result of $M_4 \cdot x^{k-1}$ and $M_4 \cdot y^{k-1}$ as presented in the lecture. Ignoring normalization, find x^{k-1} and y^{k-1}. Can you find several solutions for x^{k-1} and y^{k-1}? What is the conclusion wrt. the (non-)existence of an inverse of M_4?

Exercise 3: (From random polygons to an ellipse)
Given vector $v = (v_1, \ldots, v_5) = (0, 3, -1, 11, -3)$.

1. Determine $w = v - \overline{v}$, where $\overline{v}$ is a vector where each entry is the mean of all values v_i.

2. Determine $\frac{w}{||w||_2}$, where $|| \cdot ||_2$ refers to the 2-norm.

3. What is the length of vector $\frac{w}{||w||_2}$?

Exercise 4: (From random polygons to an ellipse, numerical issues)

1. Use python to compute 0.1 + 0.2. See `https://docs.python.org/2/tutorial/floatingpoint.html` for an introduction to understand the results your observe.

2. Study the three following examples of python code. Essentially in all three examples a function f is applied c times, and then f^{-1} is applied c times.

   (a) Which result is expected mathematically?

   (b) Without running the code: which of the three examples might suffer from numerical issues “most”?

   (c) Without running the code: for which values of c do you expect to see numerical issues?

   (d) Why is this related to the lecture “From Random Polygon to Ellipse”?

```
#Example 1
for c in range(2000):
    a=1.0
    for i in range(c):
        a=a/2

    for i in range(c):
        a=a*2

    print(c,a)

#Example 2
for c in range(2000):
    a=1.0
    for i in range(c):
        a=a/2+1.0

    for i in range(c):
        a=(a-1.0)*2

    print(c,a)

#Example 3
for c in range(2000):
    a=1.0
    for i in range(c):
        a=a/2+10000.0

    for i in range(c):
        a=(a-10000.0)*2

    print(c,a)
```