## Opgaver DM534 uge 50

Husk at læse de relevante sider i slides og noter før du/I forsøger at løse en opgave.

## I: Løses i løbet af øvelsestimerne i uge 50

1. Let the following weighted graph $G$ (from the lecture slides, weights are depicted in red) be given:


It has the following distance matrix $D$ :

$$
D=\begin{gathered}
1 \\
2 \\
3 \\
4 \\
5 \\
6 \\
6
\end{gathered}\left(\begin{array}{llllll}
1 & 2 & 3 & 4 & 5 & 6 \\
0 & 1 & 3 & 7 & 2 & 6 \\
1 & 0 & 2 & 6 & 3 & 5 \\
7 & 2 & 0 & 4 & 5 & 3 \\
2 & 3 & 4 & 0 & 6 & 1 \\
6 & 5 & 3 & 1 & 7 & 0
\end{array}\right)
$$

(a) How many shortest path in $G$ are of length 6 ? Name them.
(b) How long is the longest of all pairwise shortest paths in the graph? Are there several longest shortest paths?
(c) How many paths in $G$ are of length 6? (Note: a path does not necessarily need to be a shortest path.) Name them.
2. Assume in this exercise that all weights on edges are non-negative values.
(a) In a graph $G$ with $n=6$ vertices, how many matrix-matrix multiplication operations are needed in the worst case in order to compute the distance matrix $D$, when the method of repeated squaring is used to compute $D$ ?
(b) In a graph $G$ with $n=200$ vertices, how many matrix-matrix multiplications are needed in the worst case in order to compute the distance matrix $D$, when the method of repeated squaring is used to compute $D$ ?
(c) Can you find a graph $G$ with $n=6$ vertices, for which $W^{4} \neq W^{5}$ ? If so, depict it.
(d) Can you find a graph $G$ with $n=6$ vertices, for which $W^{5} \neq W^{6}$ ? If so, depict it.
(e) Can you find a graph $G$ with $n=6$ vertices, for which $W^{1}=W^{2}$ ? If so, depict it.
(f) What is the computational runtime in order to compute the distance matrix $D$ for a graph $G$ with $n$ vertices if the method of repeated squaring is used to compute $D$ ?
3. Consider the following molecule (it's called 2,3-Dimethylhexane, see https://en.wikipedia.org/wiki/2,3-Dimethylhexane):

(a) How many carbon atoms does this molecule have?
(b) Draw the graph $G$ corresponding to the carbon backbone of the molecule.
(c) Give the edge weight matrix $W$ for the graph $G$.
(d) Use your brain or the Java program ShortestPaths. java to infer the distance matrix. [Hint: the graph is rather simple, you won't need a program for that.]
(e) What is the Wiener Index $\mathcal{W}(G)$ ?
(f) How many shortest paths of length $3 i \rightarrow \ldots \rightarrow j$ with $i<j$ are in $G$ ?
(g) Using Wiener's method for predicting the boiling point, what is your prediction for 2,3-Dimethylhexane?
4. Assume in this exercise that all weights on edges are non-negative values. Prove the following theorem stated on the slides:

## Theorem:

If $G$ is a weighted graph with edge weight matrix $W$, and vertices with indices $1, \ldots, n$ then for each positive integer $k$ the $i j$-th entry of

$$
W^{k}=\underbrace{W \odot W \odot \ldots \odot W}_{k \text { times }}
$$

is the length of the shortest path from $i$ to $j$ using maximally $k$ edges. Prove this theorem by induction over $k$. [Hint: Use the induction proof for the theorem on counting different walks in a graph (page 33 of the slides) as a guidance. During this, you will need that if $i \rightarrow \cdots \rightarrow$ $s \rightarrow \cdots \rightarrow t \rightarrow \cdots \rightarrow j$ is a shortest path between $i$ and $j$, then the $s \rightarrow \cdots \rightarrow t$ part of the path must be a shortest path between $s$ and $t$ (give a contradiction based proof for this first).]

## II: Løses hjemme

Ingen (der er ikke flere øvelsestimer i kurset).

