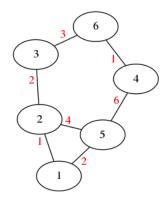
Institut for Matematik og Datalogi Syddansk Universitet, Odense 10. december 2021 DM/RF

Opgaver DM534 ug
e50

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

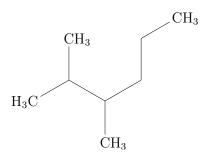
1. Let the following weighted graph G (from the lecture slides, weights are depicted in red) be given:



It has the following distance matrix D:

$$D = \begin{array}{ccccccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 0 & 1 & 3 & 7 & 2 & 6 \\ 2 & 1 & 0 & 2 & 6 & 3 & 5 \\ 3 & 2 & 0 & 4 & 5 & 3 \\ 3 & 2 & 0 & 4 & 5 & 3 \\ 7 & 6 & 4 & 0 & 6 & 1 \\ 2 & 3 & 5 & 6 & 0 & 7 \\ 6 & 5 & 3 & 1 & 7 & 0 \end{array}$$

- (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 $i \to \ldots \to j$ 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 *ij*-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 $i \to \cdots \to$ $s \to \cdots \to t \to \cdots \to j$ is a shortest path between i and j, then the $s \to \cdots \to t$ 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).