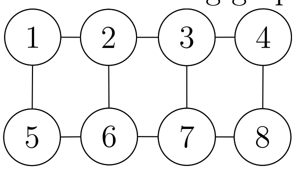
392013 Exercises Algorithmic Cheminformatics

Exercise 05. Week 23
(no mandatory exercises)

1 Cycles and Rings

Given the following graph



a) Enumerate all cycles of the graph where each node has degree 2.

b) Enumerate all simple cycles of the graph.

c) How many cycles will minimum cycle basis (MCB) have?

d) Give a MCB.

e) Give an example of a set of three linear dependent cycles.

f) Give a spanning tree which leads to a MCB.

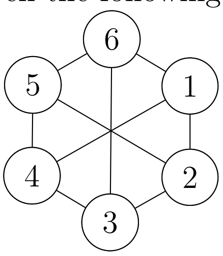
g) Give a spanning tree which does not leads to a MCB.

h) Give cycle basis which fundamental, but not strictly fundamental.

i) Give cycle basis which fundamental, but not Kirchoff-fundamental.

2 Horton's Algorithm

Given the following graph



a) Make examples of cycles in the Horton set.

b) Make an example of an elementary cycle which is not in the Horton set. Can you find a simple (i.e., chordless) cycle which is not in the Horton set?

c) What is the length of the longest cycle in the Horton set?

d) K_4 the is complete graph on four vertices with 6 undirected edges. Execute Hortons algorithm on paper and find the MCB.

3 Horton's algorithm and ChatGPT

Below is a description given by ChatGPT for Horton's algorithm, after several rounds of trying to fix mistakes. What do you think, is the below description correct?

1. **Input**: Given an undirected graph G with n vertices and m edges.
2. **Horton Set**: Compute the Horton set for the graph G. The Horton set is a set of cycles with a specific property:
   - Start with a spanning tree T of the graph G.
   - For each edge e not in the spanning tree T, find the unique cycle in $T \cup \{e\}$ (the union of T and edge e) and add it to the Horton set.
   - Repeat this process until all edges not in the spanning tree are considered.
3. **Sort the Horton Set**: Sort the cycles in the Horton set based on a specific order criterion.
4. **Minimum Cycle Basis**: The sorted Horton set forms a minimum cycle basis for the graph G.

Horton's algorithm efficiently computes a minimum cycle basis by exploiting the relationship between spanning trees and the Horton set of cycles in a graph. By sorting the cycles in the Horton set, the algorithm ensures that the resulting cycle basis is minimal.

4 Molecular Graph Invariants

Using the article [*Minimum Cycle Bases and Their Applications*, Berger, Gritzmann, Vries, 2009], determine the graph invariants for the molecules given in Fig 1:

Figure 1

5 de Pina's Algorithm

Given the following undirected graph in Fig. 2 and a spanning tree of the graph (highlighted red edges).

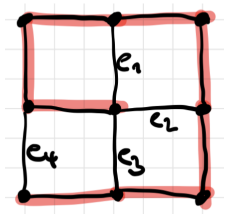


Figure 2

Assume all edges have a weight of 1. Any cycle in the cycle space can be represented as a vector

$$\mathbf{C} = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{pmatrix}$$

with $e_i \in \{0, 1\}$.

a) Which cycle is represented by $C_1 = (1, 0, 0, 0)^T$?

b) Which cycle is represented by $C_2 = (0, 0, 0, 1)^T$?

c) Which cycle-space element is represented by $C_3 = (1, 1, 1, 0)^T$?

d) Which cycle is represented by $C_4 = (0, 1, 1, 0)^T$?

e) Perform de Pina's algorithm in order to find a MCB.

f) Given the undirected graph from Fig. 3 with edge weights. What is the shortest cycle in the graph which uses an odd number of the highlighted red edges? How did you find it? Why is this question relevant to understand de Pina's algorithm?

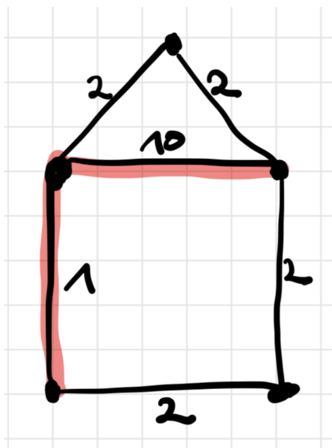


Figure 3