392013 Exercises Algorithmic Cheminformatics

Exercise 02. May 4, 2026
(no mandatory exercises)

1 Canonicalisation / Equitable Partitions

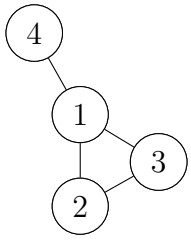
Given the following graphs, for each of them execute the equitable refinement procedure as decribed in

McKay's Canonical Graph Labeling Algorithm, Contemporary Mathematics, Stephen G. Hartke and A. J. Radcliffe, In Communicating Mathematics, volume 479 of Contemporary Mathematics, pages 99-111. American Mathematical Society, (2009).

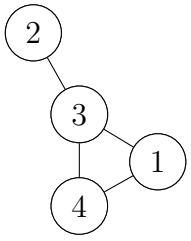
The article can be found here.

For each of the following (unlabelled) graphs give the resulting equitable partition. Note, the ids in the vertices are only representational ids, the graphs themselves are unlabelled.

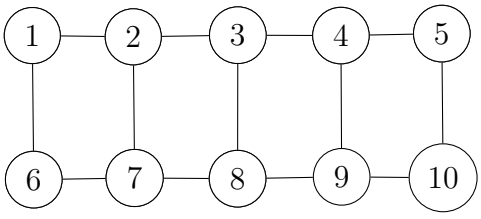
a)



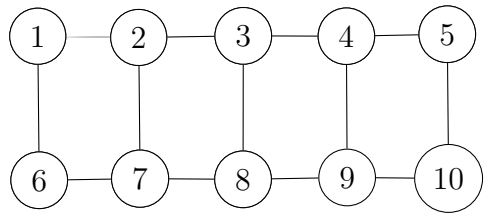
b)



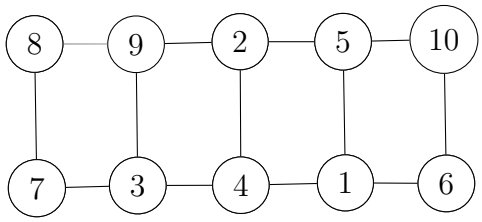
c)



d)



e)



2 Ullmann algorithm

Given the following (unlabelled) graphs G_B and G_A.

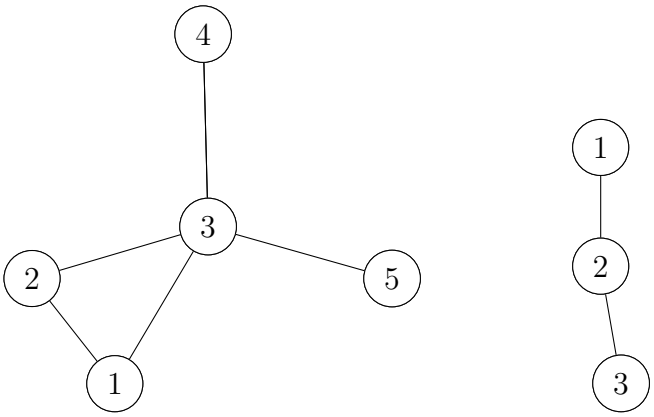


Figure 1: graph G_B (left) and graph G_A (right)

a) Give the adjacency matrices for G_A and G_B.

b) Discuss the difference between changing the adjacency condition from

$$A_{ij} = 1 \Rightarrow C_{ij} = 1 \forall i, j$$

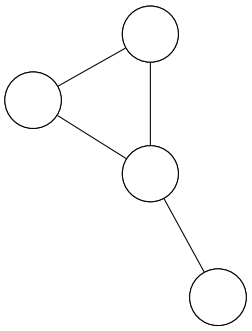
to

$$A_{ij} = 1 \Leftrightarrow C_{ij} = 1 \forall i, j$$

c) Give a matrix P (as described in the Ullmann algorithm), which acts as a certificate that G_A can be found as a monomorphism in G_B. Does your matrix P show that G_A can be found as a subgraph isomorphism in G_A? Relate your answer to question b).

3 Morgan algorithm

Given the following (unlabelled) graph G.



Execute Morgan's algorithm and specify the size of the EC classes after each iteration.