

TP n°

Machine Learning for Networks

For all exercises, try to :

- See them as some kind of research project. When coding an algorithm, think about its algorithmic complexity, other potential algorithms, why this algorithm is good or not, in which context. Test it on adequate example, potentially of different sizes.
- Use a python notebook with examples instead of just python functions.
- If asked to write a classic function (e.g. `isIsomorphic`) do not use the one from existing library. The goal for you is to understand how work the function and how to code it efficiently.

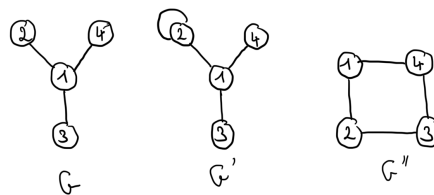
1 Assignment 3

Exercise 1 [Graph comparison. Graph kernels] The goal of the homework is to get an intuition of what are similar and not similar graphs with respect to the Random Walk Kernel. In the following, we consider a kernel function using only walks of lengths $k = 0, 1, 2, 3, 4$, that is we use the formula :

$$k_X(G, G') = \sum_{i,j=1}^{|V_X|} \left[\sum_{k=0}^4 A_X^k \right]_{ij},$$

where A_X is the adjacency matrix of the direct product graph $G \times G'$ and $|V_X|$ its number of vertices. For a matrix M , M_{ij} is the element at the intersection of line i and column j .

1. Consider the following graphs G , G' and G'' . Compute the random walk kernel value,



$k_X(G, G')$, of graphs G and G' and $k_X(G', G'')$, the random walk kernel value of graphs G' and G'' .

2. Discuss the results.
3. Play with other graphs and exhibit other triplets (at least 3 triplets) of graphs (G_1, G_2, G_3) for which G_1 and G_2 are similar and G_1 and G_3 are not.