Exercise Sheet 8

Due: 2022-12-19 12:00 o'clock

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1 Random Walk Kernels - The Weight λ

The lecture discussed the crucial role of the weight function $\lambda(l)$ in the Random Walk Kernel computation. This function defines how a walk's length influences its contribution to the kernel value. In this exercise, we consider the Geometric Random Walk Kernel as implemented in GraKeL.

1. Pick the first and second graphs of the MUTAG dataset and compare their kernel values for each $\lambda \in \{\frac{1}{10000}, \frac{1}{1000}, \frac{1}{100}, \frac{1}{10}, \frac{9}{10}\}$.
2. For each $\lambda \in \{\frac{1}{10000}, \frac{1}{1000}, \frac{1}{100}, \frac{1}{10}, \frac{9}{10}\}$, perform a 10-fold cross-validation on the MUTAG dataset and report the mean and standard deviation.
3. GraKeL provides two computation methods for the kernel which are selectable via the parameter `method_type`. Compare the runtimes for both variants for some λ.

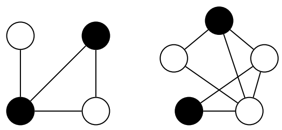
2 Random Walk Kernels - Proof

Let $\Gamma(\ell)$ be a characteristic function. and let $W_\ell(G)$ be the multiset of all walks in $G \in \mathcal{G}$ with ℓ edges. Furthermore, let $A(G)$ denote the adjacency matrix of G. Show that the following holds:

$$\sum_{\ell=0}^{\infty} \Gamma(\ell) \Big\langle W_\ell(G_1), W_\ell(G_2) \Big\rangle = \sum_{\ell=0}^{\infty} \Gamma(\ell) \Big\langle A(G_1)^\ell, A(G_2)^\ell \Big\rangle$$

3 Product Graphs

Implement a function that for two labeled graphs G and H generates the labeled direct product graph $G \times H$ (see slide 27 of lecture 8). Compute and plot the product graph of the following two graphs:



4 Kernel Design

Let k_1, k_2 be (graph) kernel functions, $G_1, G_2 \in \mathcal{G}$, and $r \in \mathbb{R}_{\geq 0}$. Show that:

1. $(r \cdot k_1)(G_1, G_2) := r \cdot k_1(G_1, G_2)$ is a kernel
2. $(k_1 + k_2)(G_1, G_2) := k_1(G_1, G_2) + k_2(G_1, G_2)$ is a kernel
3. $(k_1 \cdot k_2)(G_1, G_2) := k_1(G_1, G_2) \cdot k_2(G_1, G_2)$ is a kernel