Supplementary Material for "Studying Cerebral Vasculature Using Structure Proximity and Graph Kernels

R. Kwitt, D. Pace, M. Niethammer and S. Aylward

1 Graph-Kernel Computations

In Sect. 3 of the paper, two graph kernel values are computed for the toy example shown in Fig. 3. These kernel values are $k(\mathcal{G}_1, \mathcal{G}_2) = 11$ for the labeling scheme γ^a and $k(\mathcal{G}_1, \mathcal{G}_2) = 19$ for the labeling scheme γ^d. Eq. (1) specifies the formula for computing these kernel values:

$$k(\mathcal{G}_u, \mathcal{G}_v) = \langle [c_0(\mathcal{G}_u, l_{01}), \ldots, c_h(\mathcal{G}_u, l_{h|E_h|})], [c_0(\mathcal{G}_v, l_{01}), \ldots, c_h(\mathcal{G}_v, l_{h|E_h|})] \rangle. \tag{1}$$

1.1 Case 1: using labeling scheme γ^a

According to Fig. 4, we have 8 nodes in total which are sequentially numbered $1, \ldots, 8$. Consequently, our initial label set at $h = 0$ is $E_{h=0} := \{1, \ldots, 8\}$. The label set for $h = 1$ is $E_{h=1} := \{9, \ldots, 18\}$. $E_{h=1}$ contains the *newly* created labels after one WL iteration (see text). The following table lists the occurrences (as counted by $c_h(\mathcal{G}, l_{hj})$) for each label (label counter is j) at $h = 0$ and $h = 1$. The labels that occur in both $\mathcal{G}_1$ and $\mathcal{G}_2$ are highlighted in **bold**.

				$E_{h=0}$										$E_{h=1}$					
j	1	2	3	4	5	6	7	8	j	9	10	11	12	13	14	15	16	17	18
$c_0(\mathcal{G}_1, l_{0j})$	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	$c_1(\mathcal{G}_1, l_{1j})$	**1**	1	**1**	**1**	1	1	1	0	0	0
$c_0(\mathcal{G}_2, l_{0j})$	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	$c_1(\mathcal{G}_2, l_{1j})$	**1**	0	**1**	**1**	0	0	0	0	1	1

The scalar product in Eq. (1) can thus be written as

$$k(\mathcal{G}_1, \mathcal{G}_2) = \langle [1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 0\ 0\ 0]^\top, [1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 0\ 1\ 1\ 0\ 0\ 0\ 0\ 1\ 1]^\top \rangle = \mathbf{11}$$

1.2 Case 2: using labeling scheme γ^d

For labeling scheme γ^d the initial label set at $h = 0$, i.e., $E_{h=0} := \{1, \ldots, 6\}$ is smaller than for γ^a. In fact, label 5 occurs three times in both graphs. The label set at $h = 1$, i.e., $E_{h=1} := \{7, \ldots, 14\}$ is reduced as well. The following table lists the occurrences of each label in both graphs with common labels highlighted in **bold**.

				$E_{h=0}$							$E_{h=1}$				
j	1	2	3	4	5	6	j	7	8	9	10	11	12	13	14
$c_0(\mathcal{G}_1, l_{0j})$	**1**	**1**	**1**	**1**	**3**	**1**	$c_1(\mathcal{G}_1, l_{1j})$	**1**	**1**	**1**	**1**	**1**	**1**	1	0
$c_0(\mathcal{G}_2, l_{0j})$	**1**	**1**	**1**	**1**	**3**	**1**	$c_1(\mathcal{G}_2, l_{1j})$	**1**	0	**1**	**1**	**1**	**1**	0	1

Again, the scalar product in Eq. (1) takes the form

$$k(\mathcal{G}_1, \mathcal{G}_2) = \langle [1\ 1\ 1\ 1\ 3\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 0]^\top, [1\ 1\ 1\ 1\ 3\ 1\ 1\ 0\ 1\ 1\ 1\ 1\ 0\ 1]^\top \rangle = \mathbf{19}$$