Graph Kernels

State-of-the-Art and Future Challenges

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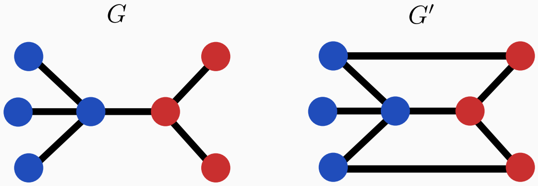
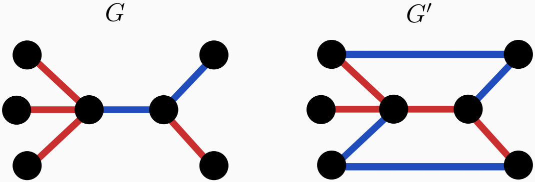
November 19, 2020

Node histogram kernel



$$\phi_{\mathrm{N}}(G) = [\; 4 \;\; 3 \;] \qquad \phi_{\mathrm{N}}(G') = [\; 4 \;\; 3 \;]$$

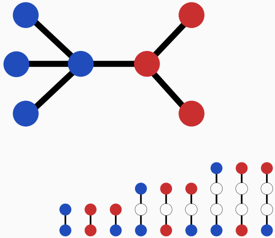
Edge histogram kernel



$\phi_{\mathrm{E}}(G) = [\ 2 \quad 4\ ]$ $\qquad$ $\phi_{\mathrm{E}}(G') = [\ 4 \quad 4\ ]$

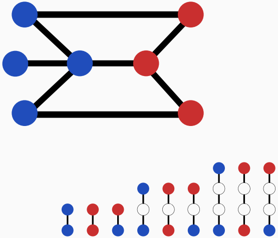
Shortest path kernel

G



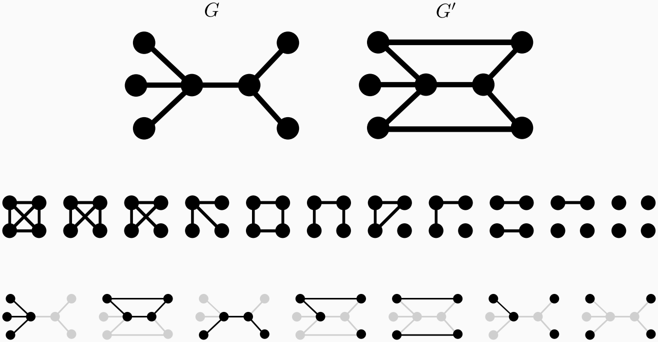
$$\phi_{\text{path}}(G) = [\,3\ \ 2\ \ 1\ \ 3\ \ 1\ \ 5\ \ 0\ \ 0\ \ 6\,]$$

G'

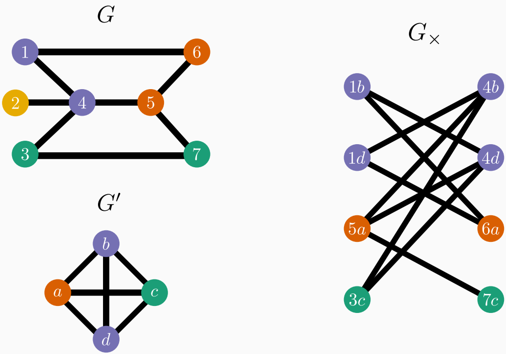


$$\phi_{\text{path}}(G') = [\,3\ \ 2\ \ 3\ \ 3\ \ 1\ \ 5\ \ 0\ \ 0\ \ 4\,]$$

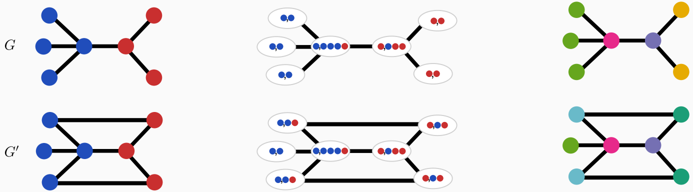
Graphlet kernel

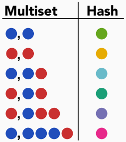


Direct product graph kernel



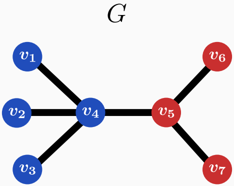
Weisfeiler–Lehman graph kernel





$\phi(G) = [\,4 \;\; 3 \;\; 3 \;\; 2 \;\; 0 \;\; 0 \;\; 1 \;\; 1\,]$ $\quad$ $\phi(G') = [\,4 \;\; 3 \;\; 1 \;\; 0 \;\; 2 \;\; 2 \;\; 1 \;\; 1\,]$

Neighbourhood hash graph kernel

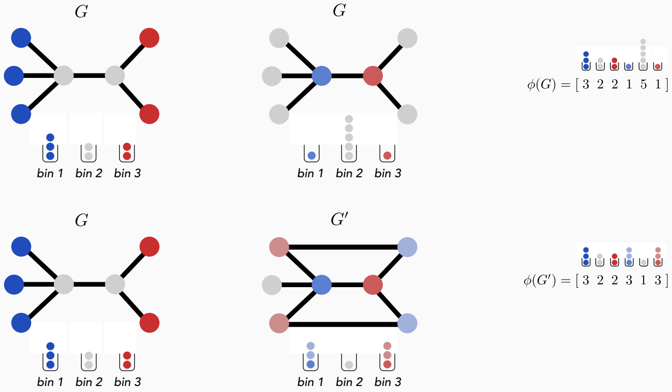


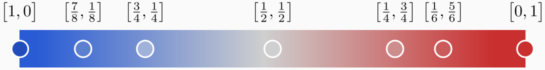
$$\ell_V(\textcolor{blue}{\bullet}) = \#1100$$
$$\ell_V(\textcolor{red}{\bullet}) = \#1110$$

$$\begin{aligned}
\mathrm{NH}(v_5) &= \mathrm{ROT}_1(\ell_V(v_5)) \oplus (\ell_V(v_4) \oplus \ell_V(v_6) \oplus \ell_V(v_7)) \\
&= \mathrm{ROT}_1(\ell_V(\textcolor{red}{\bullet})) \oplus (\ell_V(\textcolor{blue}{\bullet}) \oplus \ell_V(\textcolor{red}{\bullet}) \oplus \ell_V(\textcolor{red}{\bullet})) \\
&= \#1101 \oplus (\#1100 \oplus \#1110 \oplus \#1110) \\
&= \#0001
\end{aligned}$$

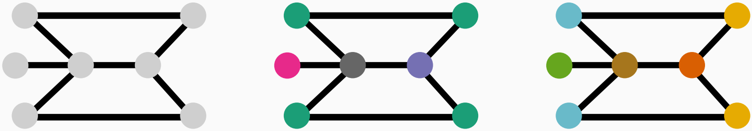
$$\begin{aligned}
\ell'_V(\textcolor{blue}{\bullet}) &= \mathrm{ROT}_1(\ell_V(\textcolor{blue}{\bullet}) \oplus \#0001) = \#1011 \\
\ell'_V(\textcolor{red}{\bullet\bullet}) &= \mathrm{ROT}_2(\ell_V(\textcolor{red}{\bullet}) \oplus \#0010) = \#0011 \\
\mathrm{CSNH}(v_5) &= \mathrm{ROT}_1(\ell(v_5)) \oplus (\ell'_V(\textcolor{blue}{\bullet}) \oplus \ell'_V(\textcolor{red}{\bullet\bullet})) \\
&= \#1101 \oplus (\#1011 \oplus \#0011) \\
&= \#0101
\end{aligned}$$

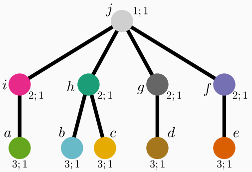
Propagation graph kernel





Weisfeiler–Lehman optimal assignment kernel





	a	b	c	d	e
a	3	1	1	1	1
b	1	3	1	1	1
c	1	1	3	2	1
d	1	1	2	3	1
e	1	1	1	1	3

$$
\begin{array}{lcllcccccccccc}
 & & & & a & b & c & d & e & f & g & h & i & j \\
\phi(\bullet) & = & \phi(a) & = [& \sqrt{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{1} & \sqrt{1} \;] \\
\phi(\bullet) & = & \phi(b) & = [& 0 & \sqrt{1} & 0 & 0 & 0 & 0 & 0 & \sqrt{1} & 0 & \sqrt{1} \;] \\
\phi(\bullet) & = & \phi(c) & = [& 0 & 0 & \sqrt{1} & 0 & 0 & 0 & 0 & \sqrt{1} & 0 & \sqrt{1} \;] \\
\phi(\bullet) & = & \phi(d) & = [& 0 & 0 & 0 & \sqrt{1} & 0 & 0 & \sqrt{1} & 0 & 0 & \sqrt{1} \;] \\
\phi(\bullet) & = & \phi(e) & = [& 0 & 0 & 0 & 0 & \sqrt{1} & \sqrt{1} & 0 & 0 & 0 & \sqrt{1} \;]
\end{array}
$$