Generalizing Weisfeiler-Lehman Kernels to Subgraphs

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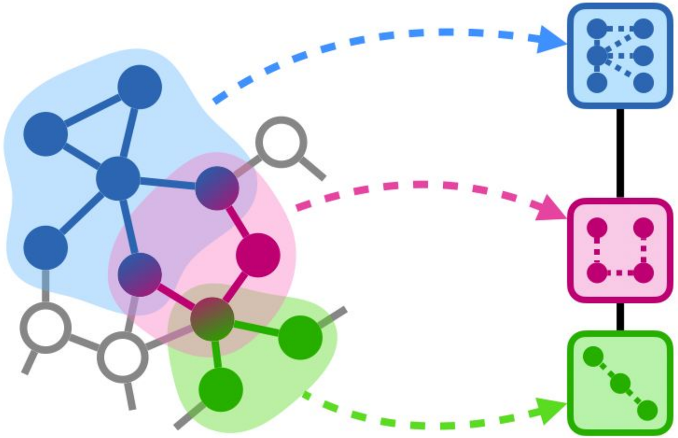

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- Example 2: Multi-hop structures around subgraphs are ***not fully encoded*** by a ***weak GNN on the whole global graph***

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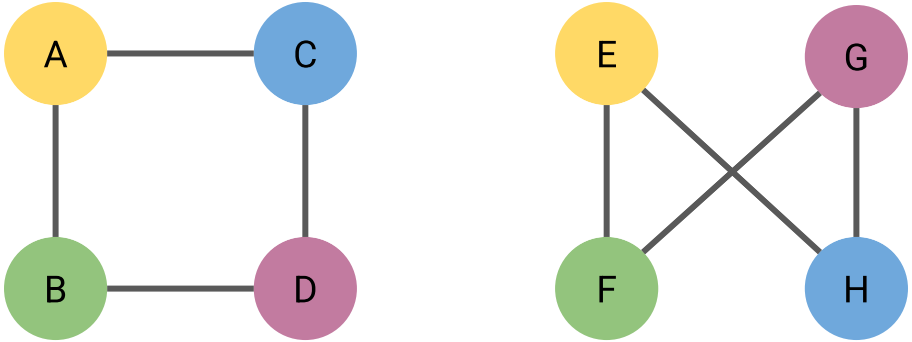
Isomorphic Graphs and the WL Test

Two graphs are ***isomorphic*** if their structures are ***identical***, meaning there is a ***one-to-one mapping between their nodes*** that preserves connectivity



Isomorphic Graphs and the WL Test

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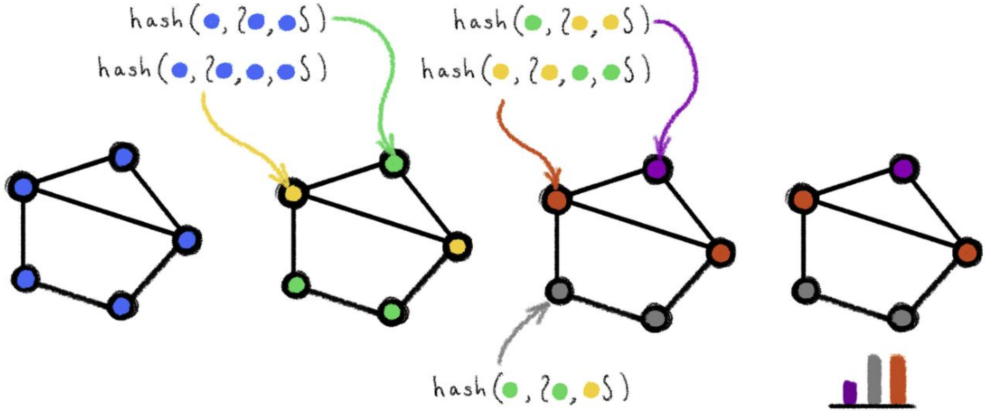
The ***WL Test*** is an efficient algorithm to distinguish ***non-isomorphic graphs*** by capturing structural difference



https://medium.com/towards-data-science/expressive-power-of-graph-neural-networks-and-the-weisefeiler-lehman-test-b883db3c7c49

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WL test on ***(k+1)-hop structures*** is ***not the same as*** WL test on ***k-hop structures***

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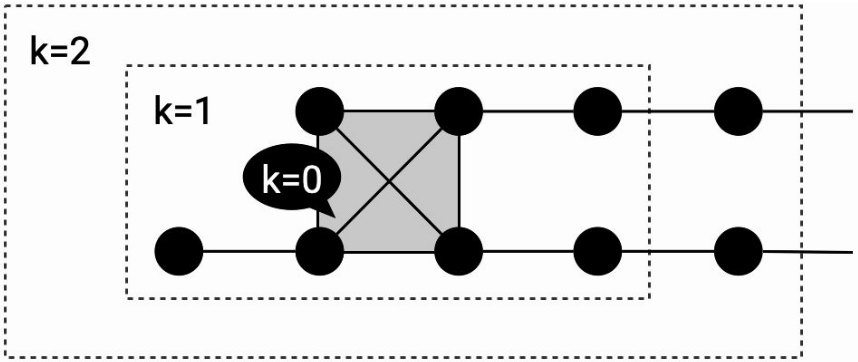
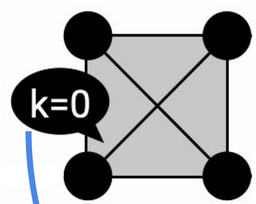
It implies that a weak K-layer GNN do not represent all the structural information of a smaller L-hop structure (L < K) from the perspective of graph isomorphism

Combining Kernels of Multi-level Structures



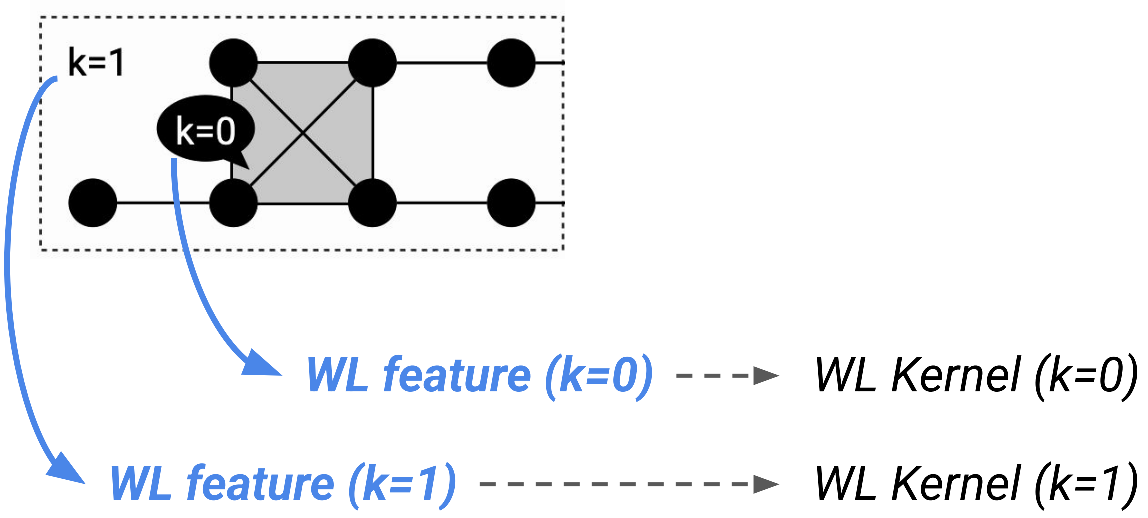
- Combining the WL test results (features) on multi-hop neighborhoods captures both local and global structures
- We use the kernel method (WL kernel) on WL features

Combining Kernels of Multi-level Structures



WL feature (k=0) - - -▶ *WL Kernel (k=0)*

Combining Kernels of Multi-level Structures



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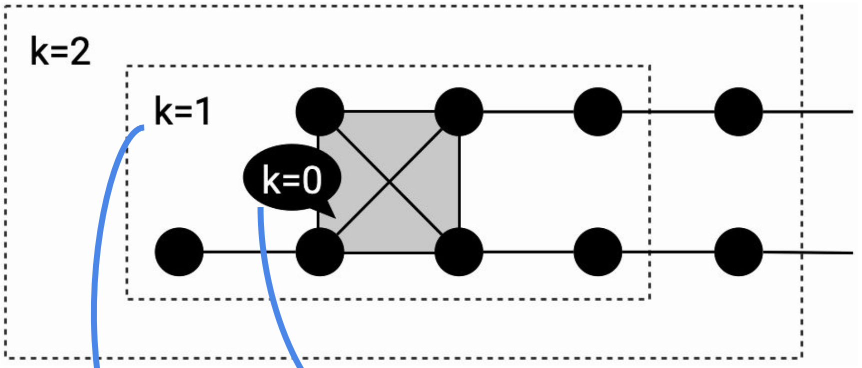

WL feature (k=0) ---> *WL Kernel (k=0)*

WL feature (k=1) ---> *WL Kernel (k=1)*

...

WL feature (k=Diameter) ---> *WL Kernel (k=D)*

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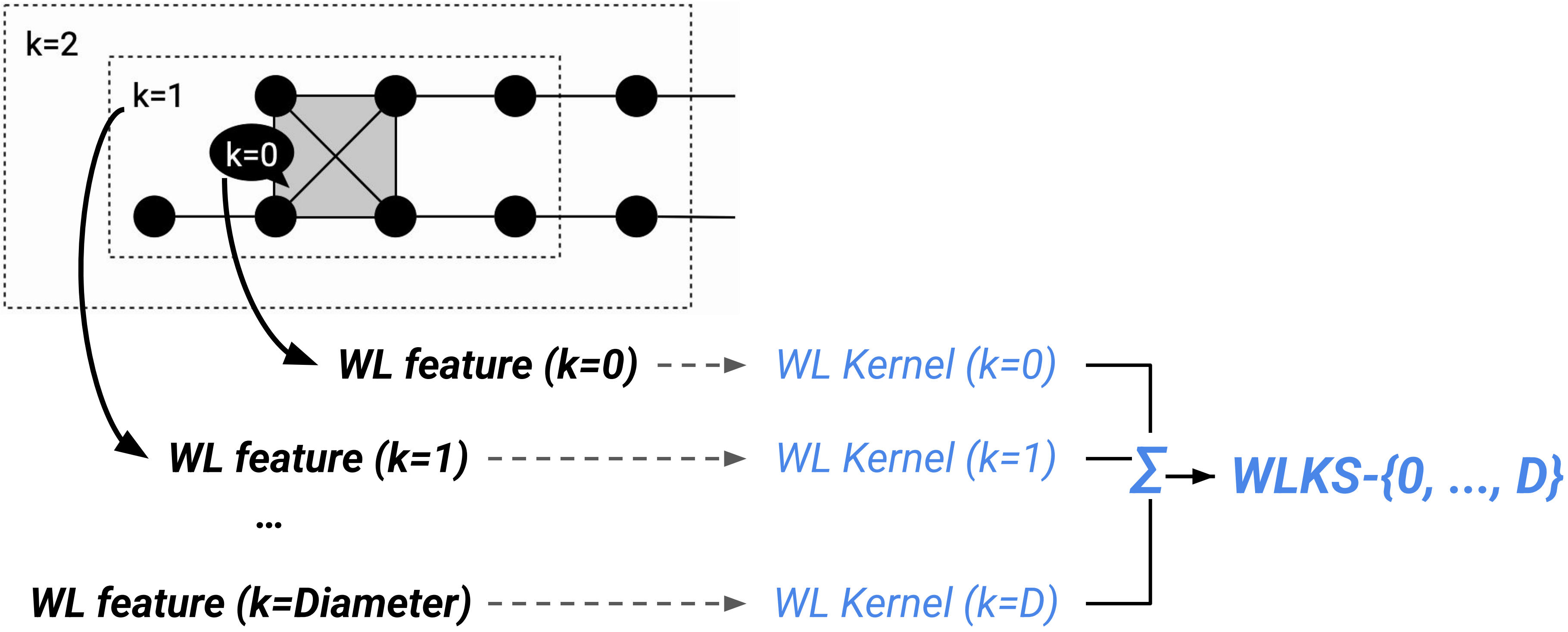

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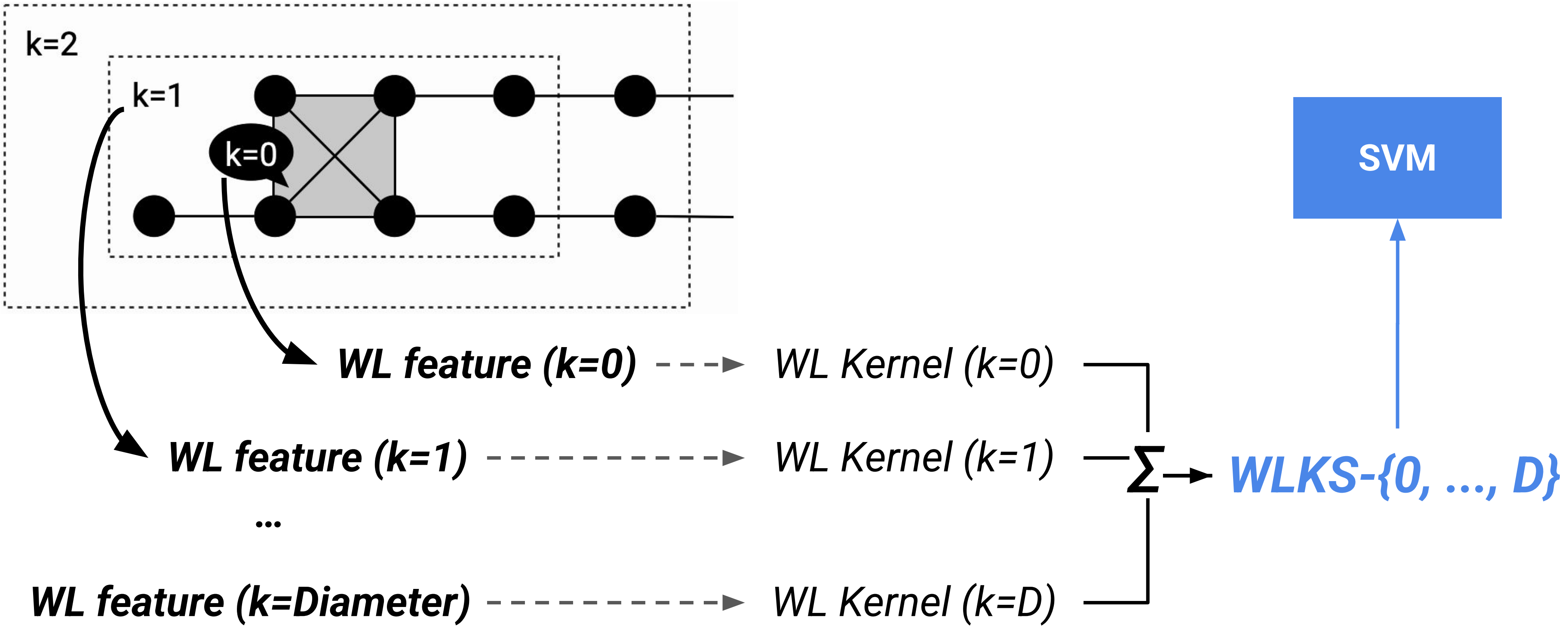

Performance of WLKS

WLKS-{0, D} outperforms the best-performing baseline in 5 out of 8 datasets

Model	PPI-BP	HPO-Neuro	HPO-Metab	EM-User	Density	Cut-Ratio	Coreness	Component
SubGNN	$59.9_{\pm 2.4}$	$63.2_{\pm 1.0}$	$53.7_{\pm 2.3}$	$81.4_{\pm 4.6}$	$91.9_{\pm 1.6}$	$62.9_{\pm 3.9}$	$65.9_{\pm 9.2}$	$95.8_{\pm 9.8}$
GLASS	$61.9_{\pm 0.7}$	$68.5_{\pm 0.5}$	$61.4_{\pm 0.5}$	$88.8_{\pm 0.6}$	$93.0_{\pm 0.9}$	$93.5_{\pm 0.6}$	$84.0_{\pm 0.9}$	$100.0_{\pm 0.0}$
VSubGAE	-	$65.2_{\pm 1.4}$	$56.3_{\pm 0.9}$	$85.0_{\pm 3.5}$	-	-	-	-
SSNP-NN	$63.6_{\pm 0.7}$	$68.2_{\pm 0.4}$	$58.7_{\pm 1.0}$	$88.8_{\pm 0.5}$	-	-	-	-
S2N+0 GCNII	$63.5_{\pm 2.4}$	$66.4_{\pm 1.1}$	$61.6_{\pm 1.7}$	$86.5_{\pm 3.2}$	$67.2_{\pm 2.4}$	$56.0_{\pm 0.0}$	$57.0_{\pm 4.9}$	$100.0_{\pm 0.0}$
S2N+A GCNII	$63.7_{\pm 2.3}$	$68.4_{\pm 1.0}$	$63.2_{\pm 2.7}$	$89.0_{\pm 1.6}$	$93.2_{\pm 2.6}$	$56.0_{\pm 0.0}$	$85.7_{\pm 5.8}$	$100.0_{\pm 0.0}$
WLKS-$\{0, D\}$	$64.8_{\pm 0.0}$	$65.3_{\pm 0.0}$	$57.9_{\pm 0.0}$	$91.8_{\pm 0.0}$	$96.0_{\pm 0.0}$	$60.0_{\pm 0.0}$	$91.3_{\pm 0.0}$	$100.0_{\pm 0.0}$

Performance of WLKS by k

WLKS-{0} and WLKS-{D} perform well independently in certain datasets, but their combination makes the better performance

Model	PPI-BP	HPO-Neuro	HPO-Metab	EM-User	Density	Cut-Ratio	Coreness	Component
WLKS-$\{0, D\}$	64.8	65.3	57.9	91.8	96.0	60.0	91.3	100.0
WLKS-$\{0\}$	34.0	31.4	26.4	67.3	96.0	36.0	87.0	100.0
WLKS-$\{1\}$	39.0	OOM	OOM	79.6	68.0	56.0	39.1	100.0
WLKS-$\{2\}$	64.2	OOM	OOM	89.8	68.0	56.0	39.1	100.0
WLKS-$\{D\}$	64.2	65.1	57.9	89.8	68.0	56.0	39.1	100.0