Wasserstein Weisfeiler-Lehman Graph Kernels

Matteo Togninalli*, Elisabetta Ghisu*, Bastian Rieck, Felipe Llinares-López, and Karsten Borgwardt
Machine Learning and Computational Biology Lab
ETH Zurich @Basel
\( R \)-Convolution kernels aggregate node representations

1. Decompose graphs in substructures
2. Compute substructure similarities
3. Average the similarities

\[
\begin{align*}
R_{\text{conv}}(a,b) & = \frac{1}{n_G n_G'} \sum_{a \in G} \sum_{b \in G'} k_{\text{base}}(a,b) \\
\end{align*}
\]
Wasserstein Weisfeiler-Lehman kernel (WWL)

1. Decompose graphs in substructures
2. Compute substructure similarities
3. Average the similarities

OLD

\[
WWL(G, G') = e^{-\lambda D_f^W(G, G')}
\]

1. Embed the graphs' nodes
2. Compute the Wasserstein Distance
3. Apply the Laplacian kernel

NEW

\[
K_{WWL}(G, G') = e^{-\lambda D_f^W(G, G')}
\]
WWL outperforms the state-of-the-art

Take home messages

- We present a novel similarity measure between graphs
- It can be used to accurately classify
  - categorically labelled graphs
  - continuously attributed and weighted graphs
- Come and see us tonight (5:00 pm – 7:00 pm)
  at poster #12
- matteo.togninalli@bsse.ethz.ch
- elisabetta.ghisu@bsse.ethz.ch