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Yusu Wang -Weisfeiler-Lehman Meets Gromov-Wasserstein

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The Weisfeiler-Lehman (WL) test is a classical procedure for graph isomorphism testing. The WL test has also been widely used both for designing graph kernels and for analyzing graph neural networks. In this talk, I will describe the so-called Weisfeiler-Lehman (WL) distance we recently introduced, which is a new notion of distance between labeled measure Markov chains (LMMCs), of which labeled graphs are special cases. The WL distance extends the WL test (in the sense that the former is positive if and only if the WL test can distinguish the two involved graphs) while at the same time it is polynomial time computable. It is also more discriminating than the distance between graphs used for defining the Wasserstein Weisfeiler-Lehman graph kernel. Inspired by the structure of the WL distance we identify a neural network architecture on LMMCs which turns out to be universal w.r.t. continuous functions defined on the space of all LMMCs (which includes all graphs) endowed with the WL distance. Furthermore, the WL distance turns out to be stable w.r.t. a natural variant of the Gromov-Wasserstein (GW) distance for comparing metric Markov chains that we identify. Hence, the WL distance can also be construed as a polynomial time lower bound for the GW distance which is in general NP-hard to compute.

This is joint work with Samantha Chen, Sunhyuk Lim, Facundo Memoli and Zhengchao Wan.