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Gromov-Wasserstein distances: Fast network comparison via entropy regularized optimal transport.

When faced with a weighted, directed network represented as a square matrix of real-valued entries (e.g. as produced by some gene regulatory network inference algorithms), further analysis is often performed by first thresholding/symmetrizing the network at some user-specified level. This is wasteful for certain tasks.

For performing retrieval, classification, or clustering on a database of networks, one implicitly needs a ground metric for comparing the networks at all threshold levels. We consider such a metric based on principles of optimal transport. A key feature of this metric is that it accounts for the significance of each node, meaning that it is robust to outliers. We provide a suite of approximate algorithms for computing this metric via entropy regularized optimal transport. These methods involve essentially only matrix-vector products, and can be easily implemented on GPU architectures for scalable, parallelized computation.

We exemplify these tools by applying them to unsupervised clustering tasks on databases of real-world and simulated networks. For the simulations, we define a generative model for random networks based on the stochastic block model that may be of independent interest. (Received September 25, 2018)