# Laplacian Global Similarity of Networks

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ABSTRACT

In this paper, we describe a methodology for comparing networks represented as weighted graphs. The key idea is to associate a probability density function derived from the graph Laplacian, and then compute the Wasserstein distance between the derived densities of the respective graphs. This has wide applications to various networks including biological and financial.

## I. INTRODUCTION

Understanding and classifying the behavior of complex systems, which can often be represented as an interconnected network, is a problem of paramount importance that arises in biology, physics, finance, and social systems [1], [2]. Such systems are rarely static and often display strong fluctuations that signify extremal events. These events, which may include cascade failures in banking ecosystems, delay propagation due to congestion in air transportation, a mutated cellular cancerous state, to even specific differentiation cellular states (e.g., muscle, bone, fat cells) derived from their parental stem cells, are usually observed through a change of topology and geometry of the underlying network. This motivates the need to view the above as dynamical system for which characterizations may elucidate certain key system-level attributes. For example, recent attempts have shown that by treating a graph as a statistical manifold, one can utilize varying geometric notions of graph curvature [3]–[5] as well as graph entropy [2], [6], [7] to understand the *functional* robustness of the system at hand with recent implications in uncovering mechanisms of drug resistance [8]. While such quantities provide valuable information in varying application settings, they are by definition, local attributes with a resolution instrinically linked at the edge and nodal scale of the network. Here, we are interested in a more global measure as seen in Figure 1. In particular, we are concerned with statistically characterizing aforementioned catalytic events based on the metric geometry comparing a *family* of networks as opposed to an individual network.

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## II. BACKGROUND AND EXAMPLES

This work focuses on first treating the eigenvalue spectrum of the normalized graph Laplacian as a probability distribution, then utilizes theory from optimal mass transport [9]–[12] to place a metric to measure distances across a family of time-varying networks. It is well-known that eigenvalue spectrum of the Laplacian provides intrinsic information of the graph. An example of a few areas that have garnered attention have included construction of expander graphs [14] to Cheeger's inequality [15] with increasing attention on connections between spectral graph theory and its respective geometry. That is, as opposed to working with the underlying discrete space alone, one can begin by placing a probability structure on a graph for which associated probability measures can be endowed with a Riemannian structure. Geodesic paths (shortest distance) ensue and convexity properties of the entropy along paths reflect on geometric qualities of the graph. It has been noted that entropy is closely related to network topology and that entropy is a selective criterion that may account for the robustness and heterogeneity of both man-made and biological networks. In particular, authors [16] previously employed a notion of *quantum entropy* based on the graph Laplacian as a measure of regularity for graphs placing it in the scope of other measures that utilize the entire spectrum (e.g., Estrada index [17]). This is in contrast to characterizing the graph towards a specific eigenvalue or its spectral gap. Following this, our work similarly takes into account the entire spectrum yet employs the $L_2$-Wasserstein distance as a measure of similarity across networks and as discussed below, its intimately related to notions of entropy.

The theory of optimal mass transport and its relationship to Riemannian geometry as well as entropy is at the core of this work. In particular, it has been recently shown [13] that the lower bounds of Ricci curvature (from geometry) are instrinically linked to Boltzmann entropy with respect $L_2$-Wasserstein metric (i.e., Ricci curvature and entropy are positively correlated). Given this, our previous work utilized a discrete notion of Ricci [3] and scalar curvature to illustrate that graph curvature may serve as a proxy for network robustness [2], [18] with distinct advantages to that network entropy [6], [7]. In the same manner, this work can be analogous viewed to that of graph quantum entropy [16]. While these parallels are briefly mentioned here (for the sake of brevity), we will revisit and note the interesting relationship between such quantities in the full manuscript.

In closing, much of this paper sets the foundation of devising various statistical methods focused on a family of networks. This can be seen in Figure 2 for which we analyze three classical graphs to illustrate the usage of our method in classifying their structure in a more global manner.

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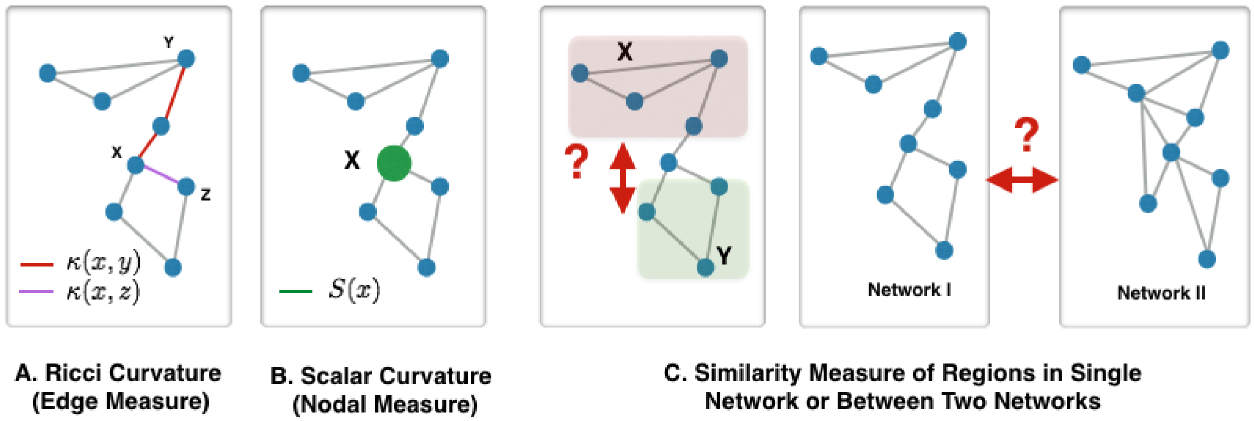


Fig. 1: There exists varying ways one can characterize a particular network. (A) Ricci curvature provides an edge measure of robustness and congestion between any two nodes . (B) Scalar curvature (via contraction of Ricci curvature) provides a nodal measure of robustness and congestion. (C) The question remains of how to properly compare two regional signaling cascades and more importantly, a family of networks characterizing a particular dynamical system.

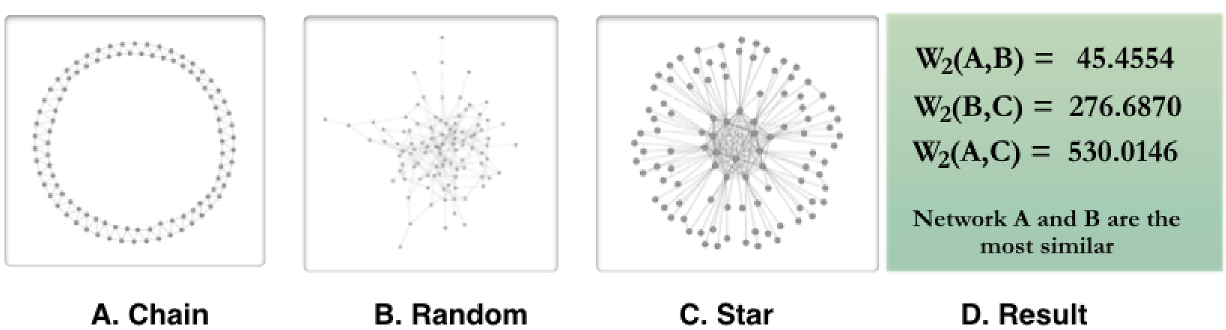


Fig. 2: We compare three classical networks and measure the $L_2$ Wasserstein distance any two given networks to illustrate a degree of similarity. Note: To avoid bias, the number of nodes (100) and edges (200) remain fixed and only the topology was allowed to change.