Length Spectrum Theory, Non-backtracking Cycles, and Two Graph Analysis Tasks

Tina Eliassi-Rad
tina@eliassi.org
Northeastern University
Boston, MA

ABSTRACT

Two basic tasks in graph analysis are: (1) computing the distance between two graphs and (2) embedding of the graph elements (i.e., nodes or links) into a lower-dimensional space. The former task has numerous applications from k -nearest neighbor search, to clustering a collection of graphs, to transfer learning. Unfortunately, there exists no canonical way of computing the distance between two finite graphs because the dissimilarity problem is ill-defined. Despite this fact, the relevant literature contains many methods for measuring graph distance with different heuristics, computational efficiency, interpretability, and theoretical soundness [1]. We introduce a graph distance, called the *Non-Backtracking Spectral Distance* (NBD), which is theoretically sound and interpretable. NBD is based on a mathematical construct from algebraic topology (in particular, homotopy) called the *length spectrum*. The length spectrum of a graph is a function defined on the graph's first homotopy group (a.k.a. *the fundamental group*); and it uniquely characterizes a graph's 2-core up to isometry [2].¹ Thus, if two graphs have the same length spectra, then their 2-cores are isometric. We show the relationship between a graph's length spectrum and its non-backtracking cycles; and present a method based on computing the eigenvalues of a graph's non-backtracking matrix. For the second task (i.e., graph embedding), most existing methods are stochastic and depend on black-box models such as deep networks. Both of these characteristics make their output difficult to analyze. We propose the *Non-Backtracking Embedding Dimensions* (NBED) for finding a graph embedding in low-dimensional space by computing the eigenvectors of the non-backtracking matrix. Both NBD and NBED are interpretable in terms of features of complex networks such as hubs, triangles, edge centrality, and communities. We showcase the usefulness of both NBD and NBED in experiments on synthetic and real-world networks.

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¹The k -core of a graph is the maximal subgraph in which each node in the subgraph has degree at least k .

CCS CONCEPTS

• **Mathematics of computing** → **Spectra of graphs**; • **Networks** → **Topology analysis and generation**; • **Computing methodologies** → *Learning latent representations*.

KEYWORDS

Graph distance, topological data analysis, length spectrum, non-backtracking matrix.

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