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On the exponential generating function for non-backtracking walks

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ABSTRACT

We derive an explicit formula for the exponential generating function associated with non-backtracking walks around a graph. We study both undirected and directed graphs. Our results allow us to derive computable expressions for non-backtracking versions of network centrality measures based on the matrix exponential. We find that eliminating backtracking walks in this context does not significantly increase the computational expense. We show how the new measures may be interpreted in terms of standard exponential centrality computation on a certain multilayer network. Insights from this block matrix interpretation also allow us to characterize centrality measures arising from general matrix functions. Rigorous analysis on the star graph illustrates the effect of non-backtracking and shows that localization can be eliminated when we restrict to non-backtracking walks. We also investigate the localization issue on synthetic networks.

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1. Introduction

1.1. Motivation

The concept of a walk on a graph is very natural—on arriving at a node, the walker may continue by traversing any edge pointing out of that node. If, at any stage, the edge along which the walker continues is the reverse of the edge on which they arrived, then the walk is said to be *backtracking*. Non-backtracking walks have been analyzed in a number of fields. They play a key role in the study of zeta functions on graphs [24], with applications in spectral graph theory [4,23], number theory [44], discrete mathematics [12,41], quantum chaos [39], random matrix theory [40], stochastic analysis [3], applied linear algebra [42] and computer science [38,45]. Within network science, constraining walks to be non-backtracking has been shown to offer benefits in community detection [26,28], centrality measurement [6,20,29,36], network comparison [30] and in the study of related issues concerning optimal percolation [31,32].

A natural task across all these fields is to count the number of distinct non-backtracking walks of a given length between pairs of nodes, and to form a compact expression for the associated generating function. For network centrality, in the case of standard walk counts it has been argued that an exponential-style power series gives a useful alternative to the standard resolvent-style version [15]. For example, based on an analogy with a physical oscillator, it may be argued that moving from the resolvent to the exponential takes us from classical to quantum physics [16]. Further, there are effective and reliable tools for computing the action of the matrix exponential [2,21,22]. This provides the initial motivation for our article, where we study the exponential generating function associated with non-backtracking walks. We also note that more general matrix functions have been proposed in this walk-counting context [17]. Hence, we then extend the analysis to cover generating functions based on arbitrary power series.

1.2. Background

We let $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ denote the adjacency matrix for an unweighted graph with n nodes; that is, $a_{ij} = 1$ if there is an edge from node i to node j, and $a_{ij} = 0$ otherwise. We will assume the graph to be loopless, so that $a_{ii} = 0$ for all i, and to have no multiple edges. If we further assume the graph represented by A to be *undirected*, i.e., if $A = A^T$, then the graph will be said to be *simple*. We use D to denote the diagonal matrix whose diagonal entries are $D_{ii} = (A^2)_{ii}$. So D_{ii} counts the number of reciprocal neighbours of node i, that is, the number of nodes j such that $a_{ij} = a_{ji} = 1$. If $A = A^T$, so that all edges are reciprocated, then D_{ii} reduces to the vector of *degrees* and any node i for which $D_{ii} = 1$ will be called a *leaf*.

If $A \neq A^T$ the network is said to be *directed* and we will denote by $S = (s_{ij}) \in \mathbb{R}^{n\times n}$ the matrix associated with the graph obtained by removing all edges that are not reciprocated, so that $s_{ij} = a_{ij}a_{ji}$ for all $i, j = 1, 2, \ldots, n$.