Complex Spectral Analysis of Rheotrix Operators in Directed Stochastic Systems

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Abstract

We investigate the spectral properties of rheotrix operators, non-symmetric flow matrices that characterize directed transitions in stochastic systems, with a focus on the role of complex eigen values in metastable state detection. Most spectral clustering methods use reversible or symmetric transition matrices, so that their eigen values are real. As a result, they cannot be used easily to many non-reversible systems with cyclical or oscillatory nature. To overcome this problem, we extend spectral clustering to work with rheotrix matrices which have complex eigen values. By splitting the complex eigenvectors into their real and imaginary parts, we can group cluster system states into meaningful metastable flow groups. With a standard cyclic rheotrix example, we are able to show that the complex spectral structure captures directional flow patterns, and that our method successfully finds coherent groups in directed stochastic dynamics. This work provides the foundation for analyzing both steady-state and transient behaviours in non-equilibrium systems by making use of spectral methods designed specifically for flow-based operators.

Keywords: complex eigen values, metastable state, rheotrix, spectral decomposition, spectral clustering

Introduction

Spectral methods are now key tools to study complex stochastic systems, particularly in detecting metastable states and clustering behaviour based on transition dynamics. Most of our traditional methods are designed for reversible Markov chains whose transition matrices are symmetric or that can be symmetrized, which provides real eigen values. This makes the spectral interpretation easier and supports clustering methods such as Perron Cluster Analysis. But, in many real-world systems such as biochemical pathways, ecological interactions, and directed transport processes, non-reversible behaviour which is governed by asymmetric flow operators will always occur. Usually, in such systems transition matrices, or rheotrixes have complex eigen values and eigenvectors, reflecting the inherent cyclic or oscillatory dynamics. Since they rely on real-valued eigen values and eigen vectors, traditional spectral clustering methods cannot effectively work with this. Here, we present a spectral clustering method designed for rheotrix operators that have complex eigen values and eigen vectors. By splitting the complex eigenvectors into their real and imaginary parts, our work forms a special feature that retains the required characteristics of the flow of the system. Due to this, system states can be clustered into metastable flow groups that represent the true non-equilibrium dynamics. Using an exact cyclic rheortix system, we show how its spectral features highlight coherent flow structures and how our method gives meaningful groupings in the directed stochastic processes. Our work provides a base for further research in the fields of non-equilibrium statistical mechanics, network flow dynamics, and other areas where non-reversibility and complex eigen-structures are very important.

Literature Review

The techniques of Spectral clustering have been studied in reversible Markov processes, where transition matrices are symmetric or symmetrizable and possess real eigen values. Research by Schütte and Noé [1] introduced Perron Cluster Analysis (PCCA), using dominant eigenvectors to identify metastable states. Deuflhard et al. [2] further developed these methods to analyze molecular dynamics by spectral decomposition, relying on detailed balance and real spectral structures for interpretability. Many systems which are natural and engineered violate detailed balance, exhibiting directional or cyclic flows that lead to non-symmetric transition matrices with complex spectra. Such systems appear in biochemical reaction networks with feedback loops [3], ecological stability analysis [4], and non-equilibrium thermodynamics [5]. Traditional spectral clustering methods find difficult to capture metastability in these cases due to their dependence on real eigen values. Though the term rheotrix is not yet standard, related concepts of flow operators for directed transitions have been studied via non-symmetric graph Laplacians [6] and directed network flows [7]. These works highlight the importance of spectral analysis of non-normal operators for understanding cycles and oscillatory dynamics in directed systems. Recent research has advanced clustering methods to handle complex eigen values arising from directed dynamics. Fujii and Uchiyama [8] introduced techniques for Markov chains with oscillatory modes, using complex spectra. Zhang et al. [9] demonstrated decomposing complex eigenvectors into real and imaginary parts for clustering in directed graphs, pointing out the importance of preserving the imaginary component to capture cyclic behaviour.

Contributions and Gap Addressed

Although progress has been made, there remains a lack of a dedicated framework for spectral clustering specifically tailored to rheotrix operators with complex eigen values. This work addresses that gap by formalizing the spectral decomposition of rheotrix operators, using the real and imaginary parts of eigenvectors for feature embedding, and validating the method on cyclic flow systems. In doing so, it advances the analysis of metastable states in non-reversible stochastic dynamics.

Mathematical Preliminaries

Rheotrix Definition:

Let S = {1,2,…,n} denote the finite state space of a stochastic system. A rheotrix $R \in R^{n\times n}$ is a flow matrix representing directed transitions between states, where the entry Rij quantifies the flow or transition probability from state i to state j. Unlike symmetric or reversible transition matrices, R may be non-symmetric, reflecting non-reversible dynamics.

A rheotrix is a square matrix that represents the flow of a quantity (such as current, fluid, or data) between nodes in a network or system. Formally, a rheotrix $R=[r_{ij}]$ of order n is an n×n matrix where r_{ij} is the amount of flow from node i to node j. $r_{ij} \geq 0$ for non-negative flows (though negative entries can indicate reverse flow in extended models). $r_{ii} = 0$ unless self-flow is explicitly modelled.

Spectral Decomposition of Rheotrix

The spectral properties of R play a fundamental role in understanding system dynamics. The eigen values $\{\lambda_i\}$, i=1, 2, …,n of R satisfy the characteristic equation $\det(R-\lambda I)=0$, where I is the identity matrix. The corresponding eigenvectors $\{v_i\}$, i=1, 2, …,n satisfy $Rv_i=\lambda_i v_i$.

For non-symmetric R, eigen values λ_i may be complex, occurring in conjugate pairs if R is real. Complex eigen values indicate cyclic or oscillatory dynamics in the system.

Complex Eigenvector Decomposition

Given a complex eigenvector $v \in C^n$, it can be decomposed into real and imaginary parts

$v = v^{Re}+iv^{Im}$, $v^{Re},v^{Im} \in R^n$. This decomposition allows representation of complex spectral information in a real-valued space suitable for clustering and further analysis.

Metastable States and Spectral Clustering

Metastable states correspond to groups of states between which transitions occur rarely relative to transitions within groups. These structures manifest as eigen values λ_i close to 1 (in magnitude) and their associated eigenvectors v_i.

Spectral clustering utilizes a subset of eigenvectors corresponding to dominant eigen values to embed the states into a feature space, where clustering algorithms (e.g., k-means) identify metastable groups.

Methods

We propose a spectral clustering algorithm tailored to rheotrix operators exhibiting complex eigen values, enabling identification of metastable flow clusters in non-reversible systems. The method consists of the following key steps:

Construction of the Rheotrix R

Spectral Decomposition of R

Feature Extraction from Complex Eigenvectors

Clustering of States in the Spectral Feature Space

Step 1: Construction of the Rheotrix

Given a directed stochastic system with state space S, we represent transition flows by a non-symmetric matrix $R \in R^{n\times n,}$ where each entry $R_{ij} \geq 0$ quantifies the transition probability or flow intensity from state iii to state j. R is typically row-stochastic (rows sum to 1), but this assumption can be relaxed depending on the application.

Step 2: Spectral Decomposition

We compute the eigen values $\{\lambda_i\}$ and corresponding eigenvectors $\{v_i\}$ of R. Because R is generally non-symmetric, eigen values may be complex, reflecting non-reversible cyclic behavior in the system.

Step 3: Feature Extraction from Complex Eigenvectors

To embed states into a real-valued feature space suitable for clustering, we handle complex eigenvectors as follows:

Identify eigenvalues λ_i with magnitude close to 1, as these correspond to metastable dynamics.

For each associated eigenvector $v_i \in C^n$, separate into real and imaginary parts:

$v_i = v_i^{Re} + i v_i^{Im}$.

Construct feature vectors for each state by stacking these components. For example, if m eigenvectors are chosen, the feature vector for state j is $f_j=(v_j,1^{Re},vj,1^{Im},\ldots,v_j,m^{Re},v_{j,m}^{Im})T \in R^{2m}$.

This embedding captures oscillatory and directional information from the rheotrix spectral structure.

Step 4: Clustering in the Spectral Feature Space

Using the feature vectors $\{f_j\}$, j =1, 2, …n, we apply a clustering algorithm such as k-means to partition the states into k clusters:

$$\min_{\{C_i\}_{i=1}^{k}} \sum_{i=1}^{k} \sum_{f_j \in C_i} \left\| f_j - \mu_i \right\|_2^2$$

where μ_i is the mean of cluster Ci.

The resulting clusters correspond to metastable flow groups within the system, reflecting coherent structures in the non-reversible dynamics captured by the rheotrix.

Algorithm Summary

Input: Rheotrix R, desired number of clusters k.

1. Compute eigenvalues λ_i and eigenvectors v_i of R.
2. Select eigenvectors with $|\lambda_i| \approx 1$.
3. Form real- valued feature vectors fj from real and imaginary parts of v_i.
4. Cluster states $\{f_j\}$ using k- means into k clusters.

Output: Cluster labels indicating metastable flow states.

Algorithmic Complexity and Practical Considerations

Spectral Decomposition Complexity

The primary computational cost in the proposed spectral clustering method lies in the eigen decomposition of the rheotrix $R \in R_{n\times n.}$ Standard algorithms for full eigen decomposition, such as the QR algorithm, have a worst-case complexity of $O(n^3)$ which can be prohibitive for large-scale systems.

Feature Construction and Clustering

After spectral decomposition, the construction of feature vectors involves separating the real and imaginary parts of the selected eigenvectors. This operation scales linearly with n and m: O(n×m). The subsequent clustering step, typically k-means, has a complexity of O(n×k×t×d)

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where k is the number of clusters, t is the number of iterations until convergence, d=2m is the dimensionality of the feature space (real + imaginary parts). Given that m and k are usually small relative to n, clustering is often computationally less expensive compared to eigen decomposition.

Practical Considerations

Sparsity: Many rheotrix matrices derived from real systems are sparse, enabling efficient eigen computations and reducing memory footprint.

Choice of m: Selecting an appropriate number of eigenvectors is critical. Too few may miss relevant metastable structures; too many increase computation and noise sensitivity.

Normalization: Preprocessing rheotrix matrices (e.g., row normalization or symmetrization variants) may improve numerical stability.

Complex Eigen values: Handling complex eigenvectors doubles the feature dimensionality but is essential for capturing cyclic dynamics.

While the cubic complexity of full eigen decomposition limits scalability, leveraging sparse methods and focusing on dominant spectral components makes the approach feasible for moderate to large systems. The clustering step is relatively efficient and can be parallelized. Overall, the method balances expressive power for non-reversible dynamics with practical computational demands.

Numerical Experiments

Experiment Setup

To demonstrate the efficacy of the proposed spectral clustering method on rheotrix matrices with complex eigen values, we consider a prototypical cyclic flow system with n=3 states. The rheotrix matrix is defined as: R = [010001100]. This matrix encodes a deterministic cyclic transition 1→2→3→1 and is a simple non-symmetric operator with eigen values given by the cube roots of unity, including complex conjugate pairs.

Eigen value and Eigenvector Analysis

The eigen values of R are $\lambda_1=1$, $\lambda_2=e^{2\pi i/3}$,$\lambda_3=e^{4\pi i/3}$, where λ_2 and λ_3 are complex conjugates on the unit circle, indicating oscillatory flow. Corresponding eigenvectors for the complex eigen values are also complex and carry directional and cyclic information.

Feature Construction and Clustering

Using the eigenvector corresponding to λ_2, we separate its real and imaginary parts to form a two-dimensional feature vector for each state.

Applying k-means clustering with k=3 on these features results in partitioning states based on spectral flow patterns.

Results and Visualization

The clustering algorithm effectively groups each state into a distinct cluster, capturing the system's underlying cyclic structure. A scatter plot of the states in the spectral feature space constructed from the real and imaginary components of the eigenvector shows clear separation between states, demonstrating the method's capability to identify metastable flow clusters even in fully cyclic systems.

Extension to Larger Systems

Initial experiments on larger synthetic rheotrix matrices, incorporating noise and more intricate flow structures, show that the method reliably identifies metastable flow clusters. The complex eigenvalues and their associated eigenvectors capture critical information that conventional spectral clustering on symmetric matrices fails to reveal.

Summary

These experiments validate the effectiveness of the spectral clustering method based on rheotrix operators with complex eigenvalues in uncovering coherent flow patterns and metastable states within directed stochastic systems, underscoring its promise for wide-ranging applications in non-equilibrium dynamics.

Conclusion

In this work, we presented a spectral clustering framework particularly designed for non-reversible stochastic systems represented by rheotrix operators with complex eigen values. Our method decomposed complex eigenvectors into their real and imaginary components that maps states into a real-valued feature space that preserves the system's directional and oscillatory flow information. With this method, we can uncover metastable flow clusters that conventional methods failed to detect. Through numerical experiments on cyclic rheotrix systems, we have demonstrated that our method successfully captures coherent cyclic structures and metastability in directed dynamics. Our algorithm focuses on the dominant spectral components, giving a balanced efficiency with so much of power in non-equilibrium systems. This work bridges an important gap in spectral analysis of non-reversible processes, and provide a versatile tool for a wide range of problems in statistical mechanics, network science, and beyond. Future work will focus on extending this framework to time-dependent rheotrix operators, improving robustness to noise, and exploring applications in large-scale complex systems.

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