Fast Incremental von Neumann Graph Entropy Computation: Theory, Algorithm, and Applications

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Abstract

The von Neumann graph entropy (VNGE) facilitates the measure of information divergence and distance between graphs in a graph sequence and has successfully been applied to various network learning tasks. Albeit its effectiveness, it is computationally demanding by requiring the full eigenspectrum of the graph Laplacian matrix. In this paper, we propose a Fast Incremental von Neumann Graph Entropy (FINGER) framework, which approaches VNGE with a performance guarantee. FINGER reduces the cubic complexity of VNGE to linear complexity in the number of nodes and edges, and thus enables online computation based on incremental graph changes. We also show asymptotic consistency of FINGER to the exact VNGE, and derive its approximation error bounds. Based on FINGER, we propose ultra-efficient algorithms for computing Jensen-Shannon distance between graphs. Our experimental results on different random graph models demonstrate the computational efficiency and the asymptotic consistency of FINGER. In addition, we also apply FINGER to two real-world applications and one synthesized dataset, and corroborate its superior performance over seven baseline graph similarity methods.

1 Introduction

In recent years, graph-based learning has become an active research field [1, 2, 3, 4, 5, 6]. Its success is rooted in the advanced capability of summarizing and representing phenomenal structural features embedded in graphs. In particular, evaluating similarity between graphs is crucial to network analysis and graph-based anomaly detection [7, 8, 9]. For example, Yanardag and Vishwanathan used graph similarity for learning novel graph kernels [10], and Sharpnack et al. proposed the Lovasz extended scan statistic for anomaly detection in connected graphs [11]. Koutra et al. proposed DeltaCon, a state-of-the-art similarity algorithm in terms of its scalability and capability of handling weighted graphs using fast belief propagation [12]. However, these methods are sensitive to heuristic metrics and presumed models, and thus provide limited understanding on the general notion of variations between graphs. On the other hand, model-agnostic approaches such as graph entropy have been used to quantify the structural complexity of a single graph, which relates to the Shannon entropy of a probability distribution over a function of enumerated subgraphs in a graph [13, 14, 15]. However, graph entropy can be computationally demanding due to its use of exhaustive subgraph search.

Different from the aforementioned approaches and inspired by quantum information theory, the von Neumann graph entropy (VNGE) [16, 17, 18] facilitates the measure of (quantum) Jensen-Shannon divergence and distance [19, 20] between graphs. It associates with a model-agnostic information measure for quantifying variation between two quantum density matrices. In addition, the VNGE has been shown to be linearly correlated with classical graph entropy measures [21, 22]. The VNGE and the Jensen-Shannon distance have been successfully applied to structural reduction in multiplex networks [23], depth analysis in image processing [24, 25], structure-function analysis in genetic networks [26], and network-ensemble comparison [27]. However, despite its effectiveness, the
compution of VNGE requires (at most) cubic complexity in the number of nodes, thereby impeding its applicability to machine learning and data mining tasks involving a sequence of large graphs.

Related Work. The VNGE was firstly defined based on the combinatorial graph Laplacian matrix \[ L \] [16, 17, 18, 23, 27]. Variants of VNGE and their approximations have been proposed in the literature, including the normalized graph Laplacian matrix \[ L_c \] proposed in [24] and the generalized graph Laplacian matrix of directed graphs [29] proposed in [30]. However, these alternatives lack approximation justification and are shown to be suboptimal in Section 2. To the best of our knowledge, this paper is the first work that provides fast VNGE computation with approximation analysis.

Contributions. To overcome the computational inefficiency of VNGE, we propose a Fast Incremental von Neumann Graph Entropy (FINGER) framework to approximate VNGE with a performance guarantee, reducing its cubic complexity to linear complexity in the number of nodes and edges. FINGER is a generic tool that applies to both batch and online graph sequences. It enables fast computation when every single graph in a graph sequence is presented (e.g., a snapshot of a dynamic network, or a single-layer connectivity pattern of a multiplex network). For applications where changes in a graph (e.g., addition and deletion of nodes or edges over time) are continuously reported (e.g., streaming graphs), FINGER also allows online computation based on incremental graph changes. We prove that FINGER maintains an approximation guarantee and is asymptotically consistent to the exact VNGE, which is further validated by different synthetic random graphs. We then apply FINGER to developing ultra-efficient algorithms for the computation of Jensen-Shannon distance between graphs. Comparing to the state-of-the-art graph similarity methods and two alternative approximate VNGE, FINGER yields superior and robust performance for anomaly detection in evolving Wikipedia networks and router communication networks, as well as bifurcation analysis in dynamic genomic networks. These applications show the effectiveness and potentials of Jensen-Shannon distance for network learning in a wide range of domains, which has not been rigorously explored owing to its high computation complexity in the absence of FINGER.

The contributions of this paper and the proposed framework (FINGER) are summarized as follows.

- Two types of approximate VNGE reducing its cubic complexity to linear complexity are proposed to support fast and incremental computation of VNGE. We derive their approximation error bounds and show asymptotic consistency relative to the exact VNGE under mild conditions.
- FINGER achieves nearly 100% reduction in computation time for VNGE of different random graph models and enables scalable Jensen-Shannon graph distance computation.
- On two real-world applications (anomaly detection and cellular bifurcation analysis) and one synthesized dataset, FINGER exhibits outstanding and robust performance over 7 baseline methods.

2 FINGER: Theory and Algorithms

2.1 Background and Preliminaries

Using terminology from quantum statistical mechanics, a density matrix \( \Phi \) describing a quantum system in a mixed state can be cast as a statistical ensemble of several quantum states. The \( n \times n \) matrix \( \Phi \) is symmetric, positive semidefinite, and satisfies trace(\( \Phi \)) = 1. The von Neumann entropy of a quantum system is defined as \( H = -\text{trace}(\Phi \ln \Phi) \) [31], where \( \ln \Phi \) denotes matrix logarithm. Let \( \{\lambda_i\}_{i=1}^n \) be the sorted eigenvalues of \( \Phi \) such that \( 0 \leq \lambda_0 \leq \ldots \leq \lambda_1 \). The definition of von Neumann entropy is equivalent to \( H = -\sum_{i=1}^n \lambda_i \ln \lambda_i \), where the convention \( \ln 0 = 0 \) is used due to \( \lim_{x \to 0^+} x \ln x = 0 \). Moreover, since \( \sum_i \lambda_i = 1 \) and \( \lambda_i \geq 0 \) for all \( i \), the von Neumann entropy can be viewed as the Shannon entropy associated with the eigenspectrum \( \{\lambda_i\}_{i=1}^n \).

We consider the class of undirected weighted simple non-empty graphs with nonnegative edge weights, denoted by \( \mathcal{G} \). Let \( G = (V, E, W) \in \mathcal{G} \) denote a single graph, where \( V \) and \( E \) denote its node and edge set with cardinality \( |V| = n \) and \( |E| = m \), respectively, and \( W \) is an \( n \times n \) matrix with entry \( W_{ij} = w_{ij} \) denoting the weight of an edge \( (i, j) \in E \). A graph sequence \( \{G_t\}_{t=1}^T \) refers to a set of \( T \) graphs indexed by \( t \in \{1, \ldots, T\} \) with known node-to-node correspondence, where \( G_t \in \mathcal{G} \) for all \( t \). The combinatorial graph Laplacian matrix of \( G \) is defined as \( L = S - W \) [32], where \( S = \text{diag}(s_1, \ldots, s_n) \) is a diagonal matrix and its diagonal entry \( s_i = \sum_{j=1}^n w_{ij} \) is the nodal strength (weighted degree) of a node \( i \in V \). Connecting the von Neumann entropy to graphs, the VNGE, denoted by \( \bar{H}(G) \), is defined by replacing \( \Phi \) with \( L_N = c \cdot L \) [16, 17, 18], where \( c = 1/\text{trace}(L) \) is a trace normalization factor. It has been proved in [17] that for any \( G \in \mathcal{G} \), \( \bar{H}(G) \leq \ln(n-1) \).
where the equality holds when $G$ is a complete graph. Note that since computing VNGE requires the entire eigenspectrum $\{\lambda_i\}_{i=1}^n$ of $L_N$, it incurs full eigenvalue decomposition on $L_N$ and has cubic complexity $O(n^3)$ \cite{15}, making it computationally infeasible for large graphs.

In what follows, we propose two types of approximate VNGE ($\hat{H}$ and $\tilde{H}$) for the exact VNGE $H$, where $\hat{H}$ and $\tilde{H}$ possess linear computation complexity and satisfy $\hat{H} \leq \tilde{H} \leq H$. Depending on the data format and problem setup, $\hat{H}$ is designed for fast computation of $H$ for a single graph, and $\tilde{H}$ is designed for online computation of $H$ based on incremental graph changes. Furthermore, we derive approximation error and prove asymptotic consistency relative to $H$ under mild conditions on the eigenspectrum $\{\lambda_i\}_{i=1}^n$ of $L_N$. Our proofs are presented in the supplementary material.

### 2.2 Approximation Analysis of von Neumann Graph Entropy

Recall that computing $H = -\sum_{i=1}^n \lambda_i \ln \lambda_i$ requires $O(n^3)$ computation complexity. To accelerate its computation, we first reduce its computation complexity by using the quadratic approximation of the term $\lambda_i \ln \lambda_i$ in $H$ via Taylor series expansion, leading to the following lemma.

**Lemma 1** (Quadratic approximation $Q$ of $H$). For any $G \in \mathcal{G}$, the quadratic approximation $Q$ of the von Neumann graph entropy $H$ via Taylor series expansion is equivalent to $Q = 1 - c^2 (\sum_{i,j} w_{ij} s_i + 2 \sum_{i,j} w_{ij})$, where $c = \frac{1}{2}$ and $S = \text{trace}(L) = \sum_{i \in V} s_i = 2 \sum_{i,j} w_{ij}$.

It is clear from Lemma 1 that $Q$ only depends on the edge weights on $G = (V, E, W)$, resulting in linear computation complexity $O(n + m)$ \cite{16}, where $|V| = n$ and $|E| = m$. We note that higher-order (beyond quadratic) approximation of $H$ is plausible at the price of less computational efficiency and possibly excessive subgraph pattern searching. For example, the cubic approximation of $H$ involves the computation of $\text{trace}(W^3)$, which relates to the sum of edge weights of every triangle in $G$. To identify the approximation accuracy and consistency of $Q$ with respect to $H$, the following theorem shows the approximation bounds on $H$ in terms of $Q$ and the eigenspectrum $\{\lambda_i\}_{i=1}^n$ of $L_N$.

**Theorem 1** (Approximation bounds on $H$). For any $G \in \mathcal{G}$, let $\lambda_{\max}$ and $\lambda_{\min}$ be the largest and smallest positive eigenvalue of $L_N$, respectively. If $\lambda_{\max} < 1$, then $-Q \ln \frac{\lambda_{\max}}{1 - \lambda_{\min}} \leq H \leq -Q \ln \frac{\lambda_{\min}}{1 - \lambda_{\min}}$. The bounds become exact and $H = \ln(n - 1)$ when $G$ is a complete graph with identical edge weight.

Note that Theorem 1 excludes the extreme case when $\lambda_{\max} = 1$, as the resulting VNGE is trivial ($H = 0$). The condition $\lambda_{\max} < 1$ holds for any graph $G \in \mathcal{G}$ having a connected subgraph with at least 3 nodes. In addition to the approximation bounds presented in Theorem 1, the corollary below further shows asymptotic consistency between $Q$ and $\frac{H}{\ln n}$ under mild conditions on $\lambda_{\max}$ and $\lambda_{\min}$.

**Corollary 1** (Asymptotic consistency of $Q$). For any $G \in \mathcal{G}$, let $n_+$ denote the number of positive eigenvalues of $L_N$. If $n_+ \sim n$ and $\lambda_{\max} \sim \lambda_{\min}$, then $\frac{H}{\ln n} \rightarrow Q$ as $n \rightarrow \infty$.

Corollary 1 suggests that the VNGE of large graphs with balanced eigenspectrum (i.e., $\lambda_{\max} \sim \lambda_{\min}$) can be well approximated by $Q$ and a factor $\ln n$. The condition of balanced eigenspectrum holds in regular and homogeneous random graphs \cite{17, 18}. Furthermore, since $n_+$ equals to $n - g$, where $g$ is the number of connected components in $G$ \cite{18}, the condition $n_+ \sim n$ holds when $g = o(n)$.

#### 2.3 FINGER-$\hat{H}$: Approximate von Neumann Graph Entropy $\hat{H}$ Using $Q$ and $\lambda_{\max}$

Based on the derived lower bound of $H$ as stated in Theorem 1, we propose the first type of approximate VNGE $\hat{H}$ using $Q$ and $\lambda_{\max}$ for any $G \in \mathcal{G}$, which is defined as

$$\hat{H}(G) = -Q \ln \lambda_{\max}. \quad (1)$$

Comparing to the lower bound $-Q \ln \frac{\lambda_{\max}}{1 - \lambda_{\min}}$ in Theorem 1, $\hat{H}$ is a looser lower bound on $H$ since $1 - \lambda_{\min} < 1$. Here we use $1 - \lambda_{\min} \approx 1$ when approximating $H$, since $\text{trace}(L_N) = \sum_{i=1}^n \lambda_i = 1$ and hence $\lambda_{\min}$ is negligible, especially for large graphs.

1. $f(n) = O(h(n))$ means $\lim_{n \rightarrow \infty} f(n) / h(n) < \infty$ and $f(n) = o(h(n))$ means $\lim_{n \rightarrow \infty} f(n) / h(n) = 0$.
2. For computing all eigenvalues of large matrices, a viable solution is direct methods, possibly with parallel eigensolvers for acceleration. The complexity for computing $\{\lambda_i\}_{i=1}^n$ of $L_N$ is $O(n^2 + \frac{n^3}{\alpha(n)})$ \cite{15}.
3. The complexity becomes $O(n^2)$ when $m = O(n^2)$ (i.e., dense graphs). In sparse graphs $m$ could be $O(n)$.
4. $f(n) \sim h(n)$ means $\lim_{n \rightarrow \infty} f(n) / h(n) = 1.$
More importantly, since \( \lambda_{\text{max}} \) is the largest eigenvalue of \( L_N \) and by definition \( L_N \) has \( n + m \) nonzero entries, the computation of \( \lambda_{\text{max}} \) only requires \( O(m + n) \) operations via power iteration methods \([34][37]\), leading to the same complexity as \( Q \). Consequently, by only acquiring \( \lambda_{\text{max}} \) instead of the entire eigenspectrum \( \{\lambda_i\}_{i=1}^n \), the computation of \( \tilde{H} \) has linear complexity \( O(m + n) \), resulting in significant computation reduction when compared with the exact VNGE \( H \), which requires cubic complexity \( O(n^3) \). In addition to computational efficiency, the following corollary shows that the approximation error of \( \tilde{H} \), defined as \( H - \tilde{H} \), decays at the rate of \( \ln n \) under the same conditions as in Corollary 1. We note that the \( o(\ln n) \) approximation error rate is nontrivial since \( H \leq \ln(n - 1) \) for any \( G \in \mathcal{G} \) \([17][35]\).

**Corollary 2** \( o(\ln n) \) approximation error of \( \tilde{H} \). For any \( G \in \mathcal{G} \), if \( n_+ \sim n \) and \( \lambda_{\text{max}} \sim \lambda_{\text{min}} \), then the scaled approximation error (SAE) \( \frac{H - \tilde{H}}{\ln n} \rightarrow 0 \) as \( n \rightarrow \infty \), implying \( H - \tilde{H} = o(\ln n) \).

### 2.4 FINGER-\( \tilde{H} \): Approximate von Neumann Graph Entropy \( \tilde{H} \) Using \( Q \) and \( s_{\text{max}} \)

The proxy \( \tilde{H} \) in Section 2.3 enables fast computation of VNGE for a single graph. As the exact online update of the eigenvalue \( \lambda_{\text{max}} \) in \( \tilde{H} \) based on incremental graph changes is challenging, we propose the second type of approximate VNGE \( \tilde{H} \) using \( Q \) and the largest nodal strength \( s_{\text{max}} = \max_{i \in V} s_i \) in a graph, which allows simple incremental computation of \( \tilde{H} \) based on graph changes but at the price of larger approximation error than that of \( \tilde{H} \). The approximate VNGE \( \tilde{H} \) is defined as

\[
\tilde{H}(G) = -Q \ln(2c \cdot s_{\text{max}}),
\]

where \( c \) is the trace normalization constant. Using the definition \( L_N = c \cdot L \) and the upper bound on the largest eigenvalue of \( L \) in \([38]\), we obtain \( \tilde{H} \leq \tilde{H} \) since \( \lambda_{\text{max}} \leq 2c \cdot s_{\text{max}} \), implying \( \tilde{H} \) is a looser lower bound on \( H \) when compared with \( \tilde{H} \). Nonetheless, the following corollary shows the approximation error of \( \tilde{H} \) also decays at the same rate \( o(\ln n) \) as \( H \).

**Corollary 3** \( o(\ln n) \) approximation error of \( \tilde{H} \). For any \( G \in \mathcal{G} \), if \( n_+ \sim n \) and \( \lambda_{\text{max}} \sim \lambda_{\text{min}} \), then the scaled approximation error (SAE) \( \frac{H - \tilde{H}}{\ln n} \rightarrow 0 \) as \( n \rightarrow \infty \), implying \( H - \tilde{H} = o(\ln n) \).

To enable incremental computation of VNGE using \( \tilde{H} \), let \( G = (V, E, W) \) and \( G' = (V', E', W') \) be any two graphs from a graph sequence. Without loss of generality we assume \( G \) and \( G' \) have a common node set \( V_c \) with \( |V_c| = n_0 \) nodes. In particular, the graph \( \Delta G = (\Delta V, \Delta E, \Delta W) \) with \( |\Delta V| = \Delta n \) and \( |\Delta E| = \Delta m \) is introduced to represent the changes made from converting \( G \) to \( G' \), denoted by \( G' = G \oplus \Delta G \). The terms \( \{\Delta s_i\}_{i \in \Delta V} \) and \( \{\Delta w_{ij}\}_{(i,j) \in \Delta E} \) denote the nodal strengths and edge weights of \( \Delta G \), respectively, and \( \Delta S = \sum_{i \in \Delta V} \Delta s_i \). Let \( Q' \) be the quadratic approximation of \( H(G') \). The theorem below shows that \( Q' \) can be efficiently updated based on \( Q \) of \( H(G) \), the values of \( s_{\text{max}} \) and \( c \) from \( G \), and \( \Delta G \), yielding competent complexity \( O(\Delta n + \Delta m) \).

**Theorem 2** (Incremental update of \( Q' \)). For any \( G, G' \in \mathcal{G} \) such that \( G' = G \oplus \Delta G \), given \( Q \), \( G \) and \( \Delta G \), the term \( Q' \) can be updated by \( Q' = \frac{Q - 1}{(1 + c\Delta S)^2} \Delta Q + 1 \), where \( \Delta Q = 2\sum_{i \in \Delta V} s_i \Delta s_i + \sum_{i \in \Delta V} \Delta s_i^2 + 4 \sum_{(i,j) \in \Delta E} w_{ij} \Delta w_{ij} + 2 \sum_{(i,j) \in \Delta E} \Delta w_{ij}^2 \) and \( \Delta c = -\frac{c^2 \Delta S}{1 + c\Delta S} \).

Furthermore, by the definition of \( \tilde{H} \) in (2), \( \tilde{H}(G \oplus \Delta G) \) can be efficiently updated by

\[
\tilde{H}(G \oplus \Delta G) = -Q' \ln[2(c + \Delta c)(s_{\text{max}} + \Delta s_{\text{max}})]
\]

(3)

given \( Q, s_{\text{max}} \) and \( c \) from \( G \), and graph changes \( \Delta G \), where \( \Delta c \) is defined in Theorem 2 and \( \Delta s_{\text{max}} \) is the maximum value of \( 0 \) and \( \max_{i \in \Delta V} (s_i + \Delta s_i) - s_{\text{max}} \). The computation complexity of \( \tilde{H}(G \oplus \Delta G) \) is \( O(\Delta n + \Delta m) \) since the incremental update formula of \( Q' \) in Theorem 2 and the computation of \( \Delta s_{\text{max}} \) only require \( O(\Delta n + \Delta m) \) operations.

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1 If \( G \) and \( G' \) have different nodes, the set \( V_c \) can be constructed by the set union \( V_c = V \cup V' \).
2 The notation \( \oplus \) denotes set additions \( V' = V \cup \Delta V, E' = E \cup \Delta E \) and matrix addition \( W' = W + \Delta W \).
2.5 Fast and Incremental Algorithms for Jensen-Shannon Distance between Graphs

One major utility of VNGE is the computation of Jensen-Shannon distance (JSdist) between any two graphs from a graph sequence. Consider two graphs $G = (\mathcal{V}_c, \mathcal{E}, \mathcal{W}) \in \mathcal{G}$ and $G' = (\mathcal{V}_c', \mathcal{E}', \mathcal{W}') \in \mathcal{G}$, and let $\overline{G} = (\mathcal{V}_c, \frac{\mathcal{E} + \mathcal{E}'}{2}, \frac{\mathcal{W} + \mathcal{W}'}{2})$ denote their averaged graph such that $\mathcal{W} = \mathcal{W} + \mathcal{W}'$. Then the Jensen-Shannon divergence between $G$ and $G'$ can be computed by $\text{JSdiv}(G, G') = H(\overline{G}) - \frac{1}{2}[H(G) + H(G')]$ [23]. Furthermore, the Jensen-Shannon distance between $G$ and $G'$ is defined as $\text{JSdist}(G, G') = \sqrt{\text{JSdiv}(G, G')}$, which has been proved to be a valid distance metric in [19][20].

The exact computation of $\text{JSdist}$ requires $O(n^3)$ computation complexity by the definition of $H$, where $|\mathcal{V}_c| = n$, which is computationally cumbersome for large graphs. To overcome its computational inefficiency, we apply the developed FINGER-$\hat{H}$ and FINGER-$\bar{H}$ to the computation of $\text{JSdist}$, as summarized in Algorithms 1 and 2.

Algorithm 1 FINGER-JSdist (Fast)

**Input:** Graphs $G$ and $G'$ from graph sequence $\mathcal{G}$

**Output:** $\text{JSdist}(G, G')$

1. Obtain $\overline{G} = \frac{G \oplus G'}{2}$ and compute $\bar{H}(G)$, $\bar{H}(G')$, and $\bar{H}(\overline{G})$ via FINGER-$\bar{H}$ from (1).

2. $\text{JSdist}(G, G') = \left( \bar{H}(\overline{G}) - \frac{1}{2} \left[ \bar{H}(G) + \bar{H}(G') \right] \right)^{1/2}$

Algorithm 2 FINGER-JSdist (Incremental)

**Input:** Graph $G$, graph changes $\Delta G$, and $\hat{H}(G)$

**Output:** $\text{JSdist}(G, G \oplus \Delta G)$

1. Compute $\hat{H}(G \oplus \Delta G)$ and $\hat{H}(G \oplus \Delta G)$ via FINGER-$\hat{H}$ from (3) and Theorem 2.

2. $\text{JSdist}(G, G \oplus \Delta G) = \left( \hat{H}(G \oplus \Delta G) - \frac{1}{2} \left[ \hat{H}(G) + \hat{H}(G \oplus \Delta G) \right] \right)^{1/2}$

If each graph $G_t$ in a graph sequence $\{G_t\}_{t=1}^T$ is given, then FINGER-JSdist (Fast) allows fast computation of $\text{JSdist}$ and features linear computation complexity inherited from $\hat{H}$. If a graph sequence is presented by sequential graph changes $\{\Delta G_t\}_{t=1}^{T-1}$ such that $G_{t+1} = G_t \oplus \Delta G_t$, then FINGER-JSdist (Incremental) allows online computation of $\text{JSdist}$ relative to the incremental graph changes. As will be demonstrated in Section 4, these two algorithms yield outstanding and robust performance in two real-world applications in terms of both effectiveness and efficiency.

3 Experiments

In this section we conducted intensive experiments on the VNGE of three kinds of synthetic random graphs to study the effects of graph size, average degree, and graph regularity on the approximation error of FINGER and its computational efficiency. The three random graph models are: (i) Erdos-Renyi (ER) model [39] - every node pair is connected independently with probability $p_{ER}$; (ii) Barabasi-Albert (BA) model [40] - the degree distribution follows a power-law distribution; and (iii) Watts-Strogatz (WS) model [41] - an initially regular ring network with independent edge rewiring probability $p_{WS}$ for simulating small-world networks. The parameter $p_{WS}$ controls the regularity of graph connectivity, and smaller $p_{WS}$ simulates more regular graphs. Since $\hat{H} \leq \bar{H} \leq H$, the approximation error (AE) is defined as $H - \hat{H}$ and $H - \bar{H}$, respectively. The scaled approximation error (SAE) is defined as $\frac{\text{AE}}{\lambda_{\text{max}}}$.

The computation time reduction ratio (CTRR) is defined as $\frac{\text{Time}(H) - \text{Time}(X)}{\text{Time}(H)}$, where $X \in \{\hat{H}, \bar{H}\}$ and $\text{Time}(Y)$ denotes the computation time for $Y \in \{ \hat{H}, \bar{H}, H \}$. All experiments (including Section 4) were conducted by Matlab R2016 on a 16-core machine with 128 GB RAM. The results in this section are averaged over 10 random trials. We also report more results in the supplementary material due to space limitation.

The effect of average degree $\overline{d}$ and graph regularity parameter $p_{WS}$. Figures 4(a) and 4(b) display the exact and the two approximate VNGE of ER and BA graphs and the corresponding CTRR under varying $\overline{d}$. When fixing the number of nodes $n$, both $\hat{H}$ and $\bar{H}$ better match $H$ as $\overline{d}$ increases, suggesting their AE decays with $\overline{d}$. Comparing their CTRR, the computation of $\hat{H}$ and $\bar{H}$ enjoys at least 97% speed-up relative to $H$. The drastic reduction in computation time can be explained by the efficient linear complexity of FINGER, as opposed to the high complexity in computing the entire eigenspectrum for calculating $H$. The CTRR of $\hat{H}$ slightly decays with $\overline{d}$ due to the growing number of nonzero entries (edges) in $L_N$, resulting in increasing operations for computing $\lambda_{\text{max}}$. Although the AE of $\hat{H}$ is always smaller than that of $\bar{H}$ due to the fact that $\hat{H} \leq \bar{H} \leq H$, the CTRR of $\hat{H}$ has
Figure 1: Performance evaluation of von Neumann graph entropy approximation in different random graph models with \( n = 2000 \) nodes under varying average degree \( \bar{d} \) and edge rewiring probability \( p_{WS} \). The approximation error of FINGER decays as \( \bar{d} \) increases or \( p_{WS} \) decreases. FINGER achieves nearly 100\% speed-up relative to the exact entropy computation.

Figure 2: Scaled approximation error (SAE) and computation time reduction ratio (CTRR) of \( \hat{H} \) via FINGER for different random graph models and varying number of nodes \( n \). The SAE of ER and WS graphs validates the \( o(\ln n) \) approximation error analysis in Corollaries 2 and 3. The CTRR attains nearly 100\% speed-up relative to \( H \) for moderate-size graphs \( (n \geq 2000) \).

The effect of graph size \( n \). Figure 2 displays the SAE of FINGER under the three random graph models when varying the number of nodes \( n \). Since the results of \( \hat{H} \) and \( \tilde{H} \) are similar, we show the SAE of \( \tilde{H} \) in Figure 2 and report the SAE of \( \hat{H} \) in the supplementary material. By the fact that ER and WS graphs have balanced eigenspectrum [42], for ER and WS models the SAE of both \( \hat{H} \) and \( \tilde{H} \) decays as \( n \) increases, which verifies the \( o(\ln n) \) approximation error as stated in Corollaries 2 and 3. On the other hand, the SAE of BA graphs is observed to grow logarithmically in \( n \) due to the existence of extreme eigenvalues (imbalanced eigenspectrum) [42, 43]. Similar to the observations from fixed-size graphs, for a fixed \( n \) the SAE decays with \( \bar{d} \) and graph regularity in all cases. In addition, the CTRR attains nearly 100\% speed-up relative to \( H \) for moderate-size graphs \( (n \geq 2000) \).

4 Applications

Here we apply FINGER to the computation of Jensen-Shannon (JS) distance between graphs (Section 2.5) in two applications and demonstrate its outstanding performance over seven baseline methods.

Anomaly detection in evolving Wikipedia hyperlink networks. Wikipedia is an online encyclopedia that allows editing and referencing between articles. By viewing an article as a node and a hyperlink as an edge, the evolution of Wikipedia forms a graph sequence \( \{G_t\}_{t=1}^T \) over time. Table I summarizes four evolving Wikipedia networks of different language settings collected in [44, 45].
We compute the dissimilarity metrics of each method and compare them with the ground truth for detecting anomaly in monthly edit changes. The anomaly statistics of ground truth and the approximate ground truth in terms of the Pearson correlation coefficient (PCC). A higher PCC suggests a better match with the ground truth for detecting anomaly. Therefore, we use the vertex/edge overlapping (VEO) dissimilarity score as the anomaly score.

The major differences are (i) unweighted v.s. weighted and (ii) w/ v.s. w/o ground truth.

Evaluation. The major differences are (i) unweighted v.s. weighted and (ii) w/ v.s. w/o ground truth. In the Wikipedia case (unweighted graphs), there is no other information for verifying the detected anomalies. Therefore, we use the vertex/edge overlapping (VEO) dissimilarity score as the anomaly score. VEO is an intuitive and properly normalized metric of anomaly for unweighted graphs, defined as

\[ \text{VEO} = \frac{2|E_1 \cap E_2|}{|E_1| + |E_2|} \]

for comparing the similarity of two samples. Here a high VEO score directly pinpoints the month when articles are edited by a relatively significant amount. In the genome case (weighted graphs), the ground-truth bifurcation instance was verified. Moreover, the genome dataset contains nonnegative edge weights. Therefore, in this case VEO is not an appropriate metric because by definition it is insensitive to edge weight changes.

Comparative methods. We compare the proposed method with the following baseline methods:

- **DeltaCon** [12]: DeltaCon uses the idea of fast belief propagation to compute graph similarity and outputs a similarity score \(\text{Sim}_{DC} \in [0, 1]\). We use \(1 - \text{Sim}_{DC}\) as the anomaly score.
- **RMD** [12]: RMD is the Matusita distance deduced from DeltaCon, which is defined as \(\frac{1}{\text{Sim}_{DC}} - 1\).
- **λ distance** [30,51]: The Euclidean distance between two sets of top \(k\) eigenvalues of a matrix. Here we use the weight matrix \(W\) (Adj.) and the graph Laplacian matrix \(L\) (Lap.), and set \(k = 6\).
- **GED** [30]: graph edit distance (GED) for undirected unweighted graphs is the number of operations (node/edge additions and removals) required to convert a graph \(G_t\) to another graph \(G_{t+1}\).
- **VNGE-NL** [24] / **VNGE-GL** [30]: Two VNGE heuristics using the normalized/generalized graph Laplacian matrix. Unlike FINGER, they lack an certified approximation error analysis.

Wikipedia results. We compute the dissimilarity metrics of each method and compare them with the approximate ground truth in terms of the Pearson correlation coefficient (PCC). A higher PCC suggests a better match with the ground truth for detecting anomaly in monthly edit changes. The PCC and computation time of each method are reported in Table 2. For illustration, the dissimilarity metrics of Wikipedia-EN are shown in Figure 3(a). The anomaly statistics of ground truth and FINGER meet the intuition that in the earlier stage the monthly evolution of Wikipedia is more drastic, and thus the monthly change is more drastic.
Bifurcation detection results. Based on the ground-truth statistic provided by [47], we compare the performance of detecting the critical bifurcation point by each method. Let $\theta_{t,t'}$ denote a dissimilarity metric between two graphs $G_t$ and $G_{t'}$ from $\{G_t\}_{t=1}^T$. For each method, the temporal difference score (TDS) proposed in [47] is used for bifurcation detection, which is defined as $\text{TDS}(t) = \frac{1}{2} [\theta_{t,t-1} + \theta_{t,t+1}]$ when $t \in \{2, \ldots, T-1\}$, and $\text{TDS}(1) = \theta_{1,2}$ and $\text{TDS}(T) = \theta_{T,T-1}$. The measurement(s) corresponding to a local minimum in TDS is detected as a bifurcation instance.

The ground-truth statistic and TDS of each method are shown in Figure 3(b). Among all the compared methods, FINGER-JSdist (Algorithm 1) is the only method that correctly detects the bifurcation point (index 6), and its TDS based on JS distance also resembles the shape of ground-truth statistic.

In the supplement, we also report synthesized anomaly detection results using another communication network dataset to corroborate the stability and effectiveness of the proposed FINGER method.

5 Conclusion

In this paper, we proposed FINGER, a novel framework for efficiently computing von Neumann graph entropy (VNGE). FINGER reduces the computation of VNGE from cubic complexity to linear complexity for a given graph, and allows online computation based on incremental graph changes. In addition to bounded approximation error, our theory shows that FINGER is guaranteed to have asymptotic consistency to the exact VNGE under mild conditions, which has been validated by extensive experiments on three different random graph models. The high efficiency of FINGER also leads to scalable network learning algorithms for computing Jensen-Shannon distance between graphs. Furthermore, we use two domain-specific applications to corroborate the efficiency and effectiveness of FINGER when compared to 7 baseline graph similarity methods. The results demonstrate the power of FINGER in tackling large network analysis and learning problems in different domains.
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Supplementary Material

A  Proof of Lemma[1]

For any real $x$ such that $0 < x < 1$, it is easy to show that the Taylor series expansion of $-x \ln x$ at 1 is $\sum_{x=1}^{\infty} \frac{(-1)^n}{x(x-1)^2}$. Applying this result to the term $-\lambda_i \ln \lambda_i$ in $H$ and taking the quadratic approximation of the series expansion gives

$$Q = \sum_{i=1}^{n} \lambda_i (1 - \lambda_i) = 1 - \sum_{i=1}^{n} \lambda_i^2$$  \hspace{1cm} (S1)

since by definition $\sum_{i=1}^{n} \lambda_i = \text{trace}(L_N) = 1$. The term $\sum_{i=1}^{n} \lambda_i^2$ in (S1) can be expressed as

$$\sum_{i=1}^{n} \lambda_i^2 = \text{trace}(L_N^2)$$  \hspace{1cm} (S2)

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} [L_N]_{ij} [L_N]_{ji}$$  \hspace{1cm} (S3)

$$(a) = \sum_{i=1}^{n} \sum_{j=1}^{n} [L_N]^2_{ij}$$

$$(b) = c^2 \left( \sum_{i=1}^{n} [L]_{ii}^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{j \neq i} [L]_{ij}^2 \right)$$  \hspace{1cm} (S4)

$$(c) = c^2 \left( \sum_{i \in V} s_i^2 + 2 \sum_{(i,j) \in E} w_{ij}^2 \right)$$, \hspace{1cm} (S5)

where $(a)$ is due to the matrix symmetry of $L_N$, $(b)$ is due to the definition that $L_N = c \cdot L$, and $(c)$ is due to the definition of $L$ such that $[L]_{ii} = s_i$, and $[L]_{ij} = w_{ij}$ when $(i,j) \in E$ and $[L]_{ij} = 0$ otherwise. Furthermore, define

$$S = \text{trace}(L) = \sum_{i=1}^{n} [L]_{ii} = \sum_{i \in V} s_i = 2 \sum_{(i,j) \in E} w_{ij}.$$  \hspace{1cm} (S6)

Using the relation $c = \frac{1}{\text{trace}(L)}$, we obtain the expression $Q = 1 - c^2 \left( \sum_{i \in V} s_i^2 + 2 \sum_{(i,j) \in E} w_{ij}^2 \right)$, where $c = \frac{1}{S}$ and $S = \sum_{i \in V} s_i = 2 \sum_{(i,j) \in E} w_{ij}$.

B  Proof of Theorem[1]

The assumption $\lambda_{\text{max}} < 1$ implies $0 < \lambda_i \leq \lambda_{\text{max}} < 1$ for all nonzero eigenvalues $\lambda_i$. Following the definition of $H$, we can rewrite $H$ as

$$H = -\sum_{i=1}^{n} \lambda_i \ln \lambda_i$$  \hspace{1cm} (S7)

$$= -\sum_{i, \lambda_i > 0} \lambda_i \ln \lambda_i$$  \hspace{1cm} (S8)

$$= -\sum_{i, \lambda_i > 0} \lambda_i (1 - \lambda_i) \frac{\ln \lambda_i}{1 - \lambda_i}$$  \hspace{1cm} (S9)

Since for all $\lambda_i > 0$, $\ln \lambda_{\text{min}} \leq \ln \lambda_i \leq \ln \lambda_{\text{max}} < 0$ and $0 < 1 - \lambda_{\text{max}} \leq 1 - \lambda_i \leq 1 - \lambda_{\text{min}} < 1$, we obtain the relation

$$-\frac{\ln \lambda_{\text{max}}}{1 - \lambda_{\text{min}}} \leq -\frac{\ln \lambda_i}{1 - \lambda_i} \leq -\frac{\ln \lambda_{\text{min}}}{1 - \lambda_{\text{max}}}.$$  \hspace{1cm} (S10)
Using $Q = \sum_{i=1}^{n} \lambda_i (1 - \lambda_i) = \sum_{i: \lambda_i > 0} \lambda_i (1 - \lambda_i)$ in (S1) and applying (S10) to (S9) yields

$$-Q \frac{\ln \lambda_{\max}}{1 - \lambda_{\min}} \leq H \leq -Q \frac{\ln \lambda_{\min}}{1 - \lambda_{\max}}.$$  \hspace{1cm} (S11)

When $G$ is a complete graph with identical edge weight $x > 0$, it can be shown that the eigenvalues of $L$ have 1 eigenvalue at 0 and $n - 1$ identical eigenvalues at $nx$ \cite{36}. Since the trace normalization constant $c = \frac{1}{\text{trace}(L)} = \frac{1}{(n-1)nx}$, the eigenvalues of $L_N = c \cdot L$ are $\lambda_n = 0$ and $\lambda_i = \frac{nx}{(n-1)nx} = \frac{1}{n-1}$ for all $1 \leq i \leq n - 1$, which implies $H = \ln(n - 1)$. It is easy to see that in this case $Q = 1 - \frac{1}{n} = 1 - \lambda_{\min} = 1 - \lambda_{\max}$ and $-\ln \lambda_{\max} = -\ln \lambda_{\min} = \ln(n - 1)$. Consequently, the bounds in (S11) become exact and $H = \ln(n - 1)$ when $G$ is a complete graph with identical edge weight.

C On the condition $\lambda_{\max} < 1$ in Theorem 1

Here we show that the condition $\lambda_{\max} < 1$ is always satisfied with any graph $G \in \mathcal{G}$ having a connected subgraph with at least 3 nodes. By definition, $\lambda_{\max} \leq 1$ since it is the largest eigenvalue of the scaled matrix $L_N = L / \text{trace}(L)$. Since any connected subgraph with at least 3 nodes will contribute to at least 2 positive eigenvalues of $L_N$ \cite{42, 52} and all eigenvalues of $L_N$ sum to 1, we have $\lambda_{\max} < 1$.

D Proof of Corollary 1

Since $\sum_{i=1}^{n} \lambda_i = 1$, the condition $\lambda_{\max} \sim \lambda_{\min}$ implies $\lambda_{\max}$ and $\lambda_{\min}$ are of the same order $\frac{1}{n}$, where $n_+$ is the number of positive eigenvalues of $L_N$. When the condition $n_+ \sim n$ also holds, then $\lambda_{\max} = \frac{a}{n}$ and $\lambda_{\min} = \frac{b}{n}$ for some constants $a, b$ such that $a \geq b > 0$, and we obtain

$$\lim_{n \to \infty} -\frac{1}{\ln n} \cdot \frac{\ln \lambda_{\max}}{1 - \lambda_{\min}} = \lim_{n \to \infty} \frac{1}{\ln n} \cdot \frac{\ln n - \ln a}{1 - \frac{b}{n}} = 1.$$  \hspace{1cm} (S12)

Similarly,

$$\lim_{n \to \infty} -\frac{1}{\ln n} \cdot \frac{\ln \lambda_{\min}}{1 - \lambda_{\max}} = 1.$$  \hspace{1cm} (S13)

Taking the limit of $\frac{H}{\ln n}$ and applying (S12) and (S13) to the bounds in (S11), we obtain

$$\lim_{n \to \infty} \frac{H}{\ln n} - Q = 0,$$  \hspace{1cm} (S14)

which completes the proof.

E Proof of Corollary 2

Following the proof of Corollary 1 if $n_+ \sim n$ and $\lambda_{\max} \sim \lambda_{\min}$, then $\lambda_{\max} = \frac{a}{n}$ and $\lambda_{\min} = \frac{b}{n}$ for some constants $a, b$ such that $a \geq b > 0$. We have

$$\lim_{n \to \infty} \frac{H - \hat{H}}{\ln n} = \lim_{n \to \infty} \frac{H}{\ln n} - Q + Q - \frac{\hat{H}}{\ln n} \hspace{1cm} \text{(S15)}$$

$$= \lim_{n \to \infty} Q - \frac{\hat{H}}{\ln n} \hspace{1cm} \text{(S16)}$$

$$= \lim_{n \to \infty} Q - Q \cdot \frac{\ln n - \ln a}{\ln n} \hspace{1cm} \text{(S17)}$$

$$= 0,$$  \hspace{1cm} (S18)

where (a) uses (S14) and (b) uses the definition of $\hat{H}$ in (1) and $\lambda_{\max} = \frac{a}{n}$. This implies the approximation error $H - \hat{H}$ decays with $\ln n$. That is, $H - \hat{H} = o(\ln n)$. 

2
Proof of Corollary 3

Let \( \mu_{\text{max}} \) denote the largest eigenvalue of the graph Laplacian matrix \( L \) of a graph \( G \in \mathcal{G} \). Then it is known that \( \frac{a}{n} s_{\text{max}} \leq \mu_{\text{max}} \leq 2s_{\text{max}}, \) where the lower bound is proved in [33] and the upper bound is proved in [33]. These bounds suggest that \( \mu_{\text{max}} \) has the same order as \( s_{\text{max}} \), i.e., \( \mu_{\text{max}} \sim s_{\text{max}} \). Since by definition \( L_N = c \cdot L \), it holds that \( \lambda_{\text{max}} = c \cdot \mu_{\text{max}} \) and hence \( \lambda_{\text{max}} \sim c \cdot s_{\text{max}} \). Following the proof of Corollary 1 if \( n_+ \sim n \) and \( \lambda_{\text{max}} \sim \lambda_{\text{min}} \), then \( \lambda_{\text{max}} = \frac{a}{n} \lambda_{\text{min}} \) for some constants \( a, b \) such that \( a > b > 0 \), and \( 2c \cdot s_{\text{max}} = \frac{a}{n} \) for some \( \gamma > 0 \) since \( \lambda_{\text{max}} \sim c \cdot s_{\text{max}} \). Similar to the proof of Corollary 2 we have

\[
\lim_{n \to \infty} \frac{H - \tilde{H}}{\ln n} = \lim_{n \to \infty} \frac{H}{\ln n} - Q + \frac{\tilde{H}}{\ln n} - Q
\]

(S19)

\[
\begin{align*}
&= (a) \lim_{n \to \infty} \frac{Q - \tilde{H}}{\ln n} \\
&= (b) \lim_{n \to \infty} Q - Q - \frac{\ln n - \ln \gamma}{\ln n} \\
&= 0,
\end{align*}
\]

(S20)

(S21)

(S22)

where \((a)\) uses (S14) and \((b)\) uses the definition of \( H \) in (2) and \( 2c \cdot s_{\text{max}} = \frac{a}{n} \). This implies the approximation error \( H - \tilde{H} \) decays with \( \ln n \). That is, \( H - \tilde{H} = o(\ln n) \).

Proof of Theorem 2

Let \( L \) and \( L' \) denote the graph Laplacian matrix of \( G \) and \( G' \), respectively, and let \( L_N = c \cdot L \) and \( L'_N = c' \cdot L' \) be the corresponding trace-normalized matrices. Since \( S = \text{trace}(L) = 2 \sum_{(i,j) \in E} w_{ij} \) and \( \Delta S = 2 \sum_{(i,j) \in \Delta E} \Delta w_{ij} \), it is easy to show that \( \text{trace}(L') = S + \Delta S = 1/c' \). We have

\[
c' - c = \frac{1}{S + \Delta S} - \frac{1}{S} = \frac{-\Delta S}{(S + \Delta S)S} = -cc' \Delta S
\]

(S23)

since \( c' = 1/\text{trace}(L') \) and \( c = 1/\text{trace}(L) \). This then implies \( c' = \frac{c}{1 + c \Delta S} \) and

\[
\Delta c = c' - c = \frac{-c^2 \Delta S}{1 + c \Delta S}.
\]

(S24)

Using the expression of quadratic approximation for VNGE in Lemma 1 and the relation that \( G' = G \oplus \Delta G \), we have

\[
Q - Q' = (c + \Delta c)^2 \left( \sum_{i \in V} (s_i + \Delta s_i)^2 + 2 \sum_{(i,j) \in E} (w_{ij} + \Delta w_{ij})^2 \right) \\
- c^2 \left( \sum_{i \in V} s_i^2 + 2 \sum_{(i,j) \in E} w_{ij}^2 \right) \\
= (2\Delta c + \Delta c^2) \left( \sum_{i \in V} s_i^2 + 2 \sum_{(i,j) \in E} w_{ij}^2 + \frac{\Delta Q}{2} \right) + c^2 \Delta Q,
\]

(S25)

(S26)

where \( \Delta Q = 2 \sum_{i \in \Delta V} s_i \Delta s_i + 2 \sum_{i \in \Delta V} s_i^2 + 2 \sum_{(i,j) \in \Delta E} w_{ij} \Delta w_{ij} + 2 \sum_{(i,j) \in \Delta E} \Delta w_{ij}^2 \), we use the convention \( \Delta s_i = 0 \) and \( \Delta w_{ij} = 0 \) when there are no changes made in the nodal strength of node \( i \) and in the weight of edge \((i, j)\) from \( G \) to \( G' \), respectively. Since \( Q = 1 - c^2 \left( \sum_{i \in V} s_i^2 + 2 \sum_{(i,j) \in E} w_{ij}^2 \right) \), replacing \( \sum_{i \in V} s_i^2 + 2 \sum_{(i,j) \in E} w_{ij}^2 \) with \( \frac{\Delta Q}{2} \) in (S26), and using the relation \( c' = c + \Delta c \) yields

\[
Q' = \left( \frac{c'}{c} \right)^2 Q - c^2 \Delta Q - \frac{2 \Delta c + \Delta c^2}{c^2}.
\]

(S27)
Figure S1: Approximation error and computation time reduction ratio (CTRR) of FINGER under different average degree $\bar{d}$ of WS model. The red solid line and blue dashed line refer to the results of $\hat{H}$ and $\tilde{H}$, respectively. Both $\hat{H}$ and $\tilde{H}$ achieve at least 97% speed-up relative to the computation of $H$ in all cases. It is observed that $\tilde{H}$ has larger approximation error than $\hat{H}$ but better CTRR.

Using the result from (S24) that $\frac{Q}{s} = \frac{1}{1 + c\Delta S}$, we can further simplify (S27) as

$$Q' = \frac{Q}{(1 + c\Delta S)^2} - \left(\frac{c}{1 + c\Delta S}\right)^2 \Delta Q - \frac{1}{(1 + c\Delta S)^2} + 1 \quad (S28)$$

$$Q' = \frac{Q - 1}{(1 + c\Delta S)^2} - \left(\frac{c}{1 + c\Delta S}\right)^2 \Delta Q + 1, \quad (S29)$$

which completes the proof.

**H. Additional Experimental Results on Synthetic Random Graphs**

The effect of average degree $\bar{d}$ on Watts-Strogatz graphs. Figure S1 displays the approximation error and computation time reduction ratio (CTRR) of FINGER-$\hat{H}$ and FINGER-$\tilde{H}$ under different average degree $\bar{d}$ of WS model, which is defined as $H - \hat{H}$ and $H - \tilde{H}$, respectively. It can be observed that when fixing $\bar{d}$, the approximation error decays with the edge rewiring probability for both $\hat{H}$ and $\tilde{H}$. In addition, for the same edge rewiring probability, larger $\bar{d}$ yields less approximation error. Using FINGER, both $\hat{H}$ and $\tilde{H}$ achieve at least 97% speed-up relative to the computation of $H$ in all cases. The approximate VNGE of $H$ always attains better CTRR than $\tilde{H}$ but at the price of larger approximation error due to the fact that $\hat{H} \leq \tilde{H} \leq H$.

Figure S2 displays the scaled approximation error (SAE) and computation time reduction ratio of $\tilde{H}$ via FINGER for WS model under varying number of nodes $n$ and two different settings of the average degree $\bar{d}$. Their behaviors are similar to the case of $\bar{d} = 50$ as displayed in Figure 2 (c).

The effect of graph size $n$ on FINGER-$\tilde{H}$. In comparison to $\hat{H}$ via FINGER in Figure 2, Figure S3 displays the SAE and CTRR of $\tilde{H}$ for the three different random graph models and varying number of nodes $n$. Consistent with the findings in Section 3, the SAE of $\tilde{H}$ for ER and WS graphs obeys the $o(\ln n)$ approximation error analysis as established in Corollary 5 since they have balanced eigenspectrum. On the other hand, the SAE of BA graphs grows logarithmically with $n$ due to imbalanced eigenspectrum. Fixing $n$, larger average degree or more graph regularity leads to less approximation error. Comparing to $\hat{H}$, the CTRR of $\tilde{H}$ attains nearly 100% speed-up relative to $H$ for relatively small-size graphs ($n \geq 1500$).
We note that in the Wikipedia application, we omit the edge direction for all methods except VNGE-GL since the resulting performance is almost identical. The implementation of VNGE-GL indeed considers the edge direction. We also note that in these two applications, the Jensen-Shannon distances of VNGE-NL and VNGE-GL are ineffective. Therefore, we use the consecutive difference of their approximate VNGE as the anomaly score, and take the absolute value of the anomaly score for anomaly ranking.

I Implementation Details for VNGE-NL and VNGE-GL

We note that in the Wikipedia application, we omit the edge direction for all methods except VNGE-GL since the resulting performance is almost identical. The implementation of VNGE-GL indeed considers the edge direction. We also note that in these two applications, the Jensen-Shannon distances of VNGE-NL and VNGE-GL are ineffective. Therefore, we use the consecutive difference of their approximate VNGE as the anomaly score, and take the absolute value of the anomaly score for anomaly ranking.
Figure S4: Anomaly detection in consecutive monthly Wikipedia hyperlink networks via different dissimilarity metrics. The corresponding computation time and Pearson correlation coefficient are reported in Table 2. Similar to the observations in Figure 3 (a), FINGER-JSdist (Fast) best aligns with the approximate ground truth for anomaly detection in all datasets. FINGER-JSdist (Incremental) has efficient computation time but less consistency (second best PCC among all methods).

Table S1: Performance comparison of Spearman’s rank correlation coefficient (SRCC) between the approximate ground truth and each method in the Wikipedia application. FINGER attains the best SRCC across all datasets.

| Datasets | FINGER-JS (Fast) | FINGER-JS (Inc.) | DeltaCon | RMD | λ dist. (Adj.) | λ dist. (Lap.) | GED | VNGE-NL | VNGE-GL |
|----------|-----------------|-----------------|---------|-----|----------------|----------------|-----|---------|---------|
| Wiki (sEN) | 0.5055 | 0.3849 | 0.4518 | 0.4518 | 0.4208 | 0.0402 | -0.1355 | -0.0542 | 0.2231 |
| Wiki (EN) | 0.7973 | 0.5039 | -0.4620 | -0.4620 | -0.3014 | -0.5981 | -0.7759 | -0.1823 | 0.4840 |
| Wiki (FR) | 0.7026 | 0.4563 | 0.2652 | 0.2652 | 0.4297 | -0.4355 | -0.6125 | -0.4792 | 0.3938 |
| Wiki (GE) | 0.6591 | 0.4930 | 0.3167 | 0.3167 | 0.3707 | -0.3434 | -0.5695 | -0.0156 | 0.2606 |

**J Additional results for anomaly detection in evolving Wikipedia hyperlink networks**

Additional Wikipedia network plots. The plots of dissimilarity (anomaly) metrics of different methods in Section 4 for consecutive monthly hyperlink networks of Wikipedia-sEN, Wikipedia-FR, and Wikipedia-GE are shown in Figure S4. Their performance in terms of the computation time and Pearson correlation coefficient are reported in Table 2. Similar to the observations in Figure 3 (a), FINGER-JSdist (Fast) best aligns with the approximate ground truth for anomaly detection in all datasets. FINGER-JSdist (Incremental) has efficient computation time but less consistency (still attains second best PCC among all methods).

Rank correlation coefficients. In addition to PCC, we further use the Spearman’s rank correlation coefficient (SRCC) to evaluate the consistency of each method with the approximate ground truth in this task. The results are summarized in Table S1. Similar to the results using PCC, FINGER-JS (Fast) attains the best SRCC among all the compared methods in the four Wikipedia networks. This result again confirms that JS distance via FINGER indeed learns the similar notion of anomaly as indicated by the approximate ground truth.
Figure S5: Chromatin contact matrix from Hi-C over a time course of 12 samples, which correspond to -48 hour (hr), 0 hr, 8 hr, . . . , 80 hr over 6 days.

**K Addition descriptions for bifurcation detection of cell reprogramming in dynamic genomic networks**

Genome architecture is important in studying cell development, but its dynamics and role in determining cell identity are not well understood. Myogenic differentiation 1 (MYOD1) is a master transcription factor that directly converts human fibroblasts to myogenic cells as studied in [54, 55]. Very recently, Liu et al. [47] studied the chromatin contact map (genome-wide structure) through chromosome conformation capture (Hi-C) during the conversion of human fibroblasts to myogenic cells. To understand cell reprogramming, one major question is detecting when the phase transition occurs for cell identity conversion. Liu et al. conducted experiments and constructed a 1Mb binned chromatin contact matrix (namely, Hi-C matrix) of dimension 2894 over a 6-day time course, leading to 12 sampled measurements. It was found that there exists a bifurcation point at the 6th sample (the measurement at 32 hour), suggesting that the cell reprogramming can be interpreted as a genome-wide dynamic system [56] (i.e., a graph sequence) as displayed in Figure S5, where the bifurcation occurs when a small structure change made to the cellular system causes a significant system-wide change for genome.

Liu et al. further used complex graph analysis techniques involving the temporal difference score (TDS) and multiple graph centrality features [57] to construct a representative statistic for expressing the states of the studied dynamic genomic contact network as displayed in Figure 3(b), which is used in this paper as the ground-truth statistic for comparing the performance of detecting bifurcation point using different dissimilarity and distance metrics. In particular, given the TDS of a graph dissimilarity method over measurements, a bifurcation point is defined as the saddle point of the TDS curve excluding the first and last measurements (i.e., $t = 1$ and $t = T$). The detected bifurcation point(s) of each method is displayed in Figure 3(b).

**I Synthesized Anomaly Detection Results on Dynamic Communication Networks**

To further verify the power of JS distance using the proposed FINGER method, in addition to the Wikipedia and genome datasets, we use another real-world dynamic peering network dataset at the autonomous system (AS) level (the Oregon-1 dataset [58]) to synthesize anomalous connectivity patterns that mimic the denial-of-service (DoS) attacks. Here each graph represents the router connectivity over a certain time period, leading to 9 such graphs. We synthesize anomalous events by
Table S2: Detection rate on synthesized anomalous events in the dynamic communication network.

| DoS attack (X%) | FINGER -JS (Fast) | FINGER -JS (Inc.) | DeltaCon | RMD | λ dist. (Adj.) | λ dist. (Lap.) | GED | VNGE -NL | VNGE -GL |
|----------------|-------------------|-------------------|----------|-----|----------------|----------------|-----|----------|----------|
| 1%             | 24%               | 10%               | 14%      | 14% | 24%            | 14%            | 22% | 22%      |          |
| 3%             | 75%               | 62%               | 58%      | 58% | 12%            | 14%            | 22% | 22%      |          |
| 5%             | 90%               | 77%               | 90%      | 90% | 12%            | 28%            | 41% | 67%      |          |
| 10%            | 91%               | 91%               | 91%      | 91% | 91%            | 81%            | 91% | 91%      |          |

first selecting one graph from the first 8 graphs at random, and then connecting $X\%$ of nodes to a randomly chosen node in the selected graph. This synthesized connection pattern mimics that of the DoS attack, in which multiple nodes (e.g., a botnet) aim to connect to the target node simultaneously. The task is to detect this synthesized anomalous event by comparing consecutive graphs. Table S2 reports the detection rate of different methods, where the detection rate is defined as the fraction of 100 random instances in which the anomalous event appears in the top-2 ranking based on a dissimilarity metric. Tested on $X = \{1, 3, 5, 10\}\%$, FINGER-JS (Fast) consistency attains the best detection rate among all methods, suggesting the stability and superiority of the proposed method. On the other hand, the compared methods do not always attain the best detection rate across different $X$ values. When $X$ is small (i.e., the more challenging case for detection), the detection performance of FINGER is more sensible than other methods. As $X$ becomes large, which means the DoS attack pattern is more apparent, the detection performance becomes similar.