SAGMAN: <u>S</u>TABILITY <u>A</u>NALYSIS OF <u>G</u>RAPH NEURAL NETWORKS ON THE <u>MAN</u>IFOLDS

Anonymous authors

Paper under double-blind review

ABSTRACT

Modern graph neural networks (GNNs) can be sensitive to changes in the input graph structure and node features, potentially resulting in unpredictable behavior and degraded performance. In this work, we introduce a spectral framework known as SAGMAN for examining the stability of GNNs. This framework assesses the distance distortions that arise from the nonlinear mappings of GNNs between the input and output manifolds: when two nearby nodes on the input manifold are mapped (through a GNN model) to two distant ones on the output manifold, it implies a large distance distortion and thus a poor GNN stability. We propose a distance-preserving graph dimension reduction (GDR) approach that utilizes spectral graph embedding and probabilistic graphical models (PGMs) to create lowdimensional input/output graph-based manifolds for meaningful stability analysis. Our empirical evaluations show that SAGMAN effectively assesses the stability of each node when subjected to various edge or feature perturbations, offering a scalable approach for evaluating the stability of GNNs, extending to applications within recommendation systems. Furthermore, we illustrate its utility in downstream tasks, notably in enhancing GNN stability and facilitating adversarial targeted attacks.

030

025

004

006

007 008 009

010 011

012

013

014

015

016

017

018

019

021

1 INTRODUCTION

031 The advent of Graph Neural Networks (GNNs) has sparked a significant shift in machine learning 032 (ML), particularly in the realm of graph-structured data (Keisler, 2022; Hu et al., 2020; Kipf & 033 Welling, 2016; Veličković et al., 2017; Zhou et al., 2020). By seamlessly integrating graph structure 034 and node features, GNNs yield low-dimensional embedding vectors that maximally preserve the graph structural information (Grover & Leskovec, 2016). Such networks have been successfully deployed in a broad spectrum of real-world applications, including but not limited to recommendation systems (Fan et al., 2019), traffic flow prediction (Yu et al., 2017), chip placement (Mirhoseini 037 et al., 2021), and social network analysis (Ying et al., 2018). However, the enduring challenge in the deployment of GNNs pertains to their stability, especially when subjected to perturbations in the graph structure (Sun et al., 2020; Jin et al., 2020; Xu et al., 2019). Recent studies suggest that 040 even minor alterations to the graph structure (encompassing the addition, removal, or rearrangement 041 of edges) can have a pronounced impact on the performance of GNNs (Zügner et al., 2018; Xu 042 et al., 2019). This phenomenon is particularly prominent in tasks such as node classification (Yao 043 et al., 2019; Veličković et al., 2017; Bojchevski & Günnemann, 2019). The concept of stability here 044 transcends mere resistance to adversarial attacks, encompassing the network's ability to maintain consistent performance despite inevitable variations in the input data (graph structure and node features). 046

In the literature, while there are studies primarily focused on developing more stable GNN architectures (Wu et al., 2023; Zhao et al., 2024; Song et al., 2022; Gravina et al., 2022), a few attempts to analyze GNN stability comprehensively. Specifically, (Keriven et al., 2020) first studied the stability of graph convolutional networks (GCN) on random graphs under small deformation. Later, (Gama et al., 2020) and (Kenlay et al., 2021) explored the robustness of various graph filters, which are then used to measure the stabilities of the corresponding (spectral-based) GNNs. However, these prior methods are limited to either synthetic graphs or specific GNN models. Recent survey papers, such as (Dai et al., 2024), highlight the critical role of stability analysis in trustworthy GNNs.

054 In this work, we present SAGMAN, a novel framework devised to quantify the stability of GNNs through individual nodes. This is accomplished by assessing the resistance-distance distortions 056 incurred by the nonlinear map (GNN model) between low-dimensional input and output graph-based 057 manifolds. It is crucial to note that this study aims to offer significant insights for understanding 058 and enhancing the stability of GNNs. While most robustness techniques focus on enhancing overall model robustness through architectural modifications or training strategies, they often lack finegrained, node-level stability assessments. In contrast, SAGMAN introduces a spectral framework that 060 quantifies stability at the individual node level, enabling targeted interventions such as precise attacks 061 or tailored stability enhancements. The key technical contributions of this work are outlined below: 062

• This study introduces a spectral framework (SAGMAN) for measuring the stability of GNN models 064 at the node level. This is achieved by effectively assessing the distance distortions caused by the maps between the input and output smooth manifolds. 065

• To construct the input smooth manifold for stability analysis in SAGMAN, we introduce a nonlinear graph dimension reduction (GDR) framework to transform the original input graph (with node features) into a low-dimensional graph-based manifold that can well preserve the original graph's spectral properties, such as effective resistance distances between nodes.

• SAGMAN has been empirically evaluated and shown to be effective in assessing the stability of 071 individual nodes across various GNN models in realistic graph datasets. Moreover, SAGMAN allows 072 for more powerful adversarial targeting attacks and greatly improving the stability (robustness) of the 073 GNNs. 074

 SAGMAN has a near-linear time complexity and its data-centric nature allows it to operate across various GNN variants, independent of label information, network architecture, and learned parameters, demonstrating its wide applicability.

077 079

080

081

082

083

084

085

087 880

090

075

076

063

066

067

068

069

2 BACKGROUND

STABILITY ANALYSIS OF ML MODELS ON THE MANIFOLDS 2.1

The stability of a machine learning (ML) model refers to its ability to produce consistent outputs despite small variations or noise in the input data (Szegedy et al., 2013). To assess this stability, we utilize the Distance Mapping Distortion (DMD) metric (Cheng et al., 2021). For two input data samples p and q, the DMD metric $\delta^M(p,q)$ is defined as the ratio of their distance on the output manifold to the one on the input manifold:

$$\delta^M(p,q) \stackrel{\text{def}}{=} \frac{d_Y(p,q)}{d_X(p,q)}.$$
(1)

By evaluating $\delta^M(p,q)$ for each pair of data samples, we can assess the stability of the ML model. 091 Specifically, if two nearby data samples on the input manifold are mapped to distant points on the 092 output manifold, this indicates a large $\delta^M(p,q)$ or equivalently a large local Lipschitz constant, and 093 thus poor stability of the model near these samples; On the other hand, a small $\delta^M(p,q)$ implies that 094 the model is stable in that region. 095

096 2.2 Previous Investigations on the Stability of GNNs

098 The stability of a GNN refers to its output stability in the presence of edge/node perturbations (Sun 099 et al., 2020). This includes maintaining the fidelity of predictions and outcomes when subjected to 100 changes such as edge alterations or feature attacks. A desired GNN model is expected to exhibit 101 good stability, wherein every predicted output or the graph embeddings do not change drastically in 102 response to the aforementioned minor perturbations (Jin et al., 2020; Zhu et al., 2019). Several recent 103 studies have underlined the importance of analyzing the stability of GNNs. For instance, Sharma 104 et al. (2023) examined the task and model-agnostic vulnerabilities of GNNs, demonstrating that these 105 networks remain susceptible to adversarial perturbations regardless of the specific downstream tasks. Furthermore, Huang et al. (2023) investigated robust graph representation learning via predictive 106 coding, proposing a method that enhances GNN stability by reconstructing input data to mitigate the 107 effects of adversarial attacks.

Moreover, while recent studies have investigated the stability issues of Graph Neural Networks (GNNs) on synthetic graphs or specific models (Keriven et al., 2020; Kenlay et al., 2021), they have not provided a unified framework for evaluating GNN stability. The latest state-of-the-art method (Li et al., 2024) develops such a unified framework but does not consider feature perturbations. This omission leaves a significant gap in understanding how GNNs respond to changes in node features, which is crucial for applications where feature data may be noisy or subject to perturbations.

3 THE SAGMAN FRAMEWORK FOR STABILITY ANALYSIS OF GNNS

Challenges in Applying DMD Metrics to GNN Stability Analysis. When adopting the DMD metric for the stability analysis of GNN models, a natural approach is to use graph-based manifolds (details in Appendix A.1) for calculating DMDs. However, directly using the input graph structure as the input graph-based manifold may not produce satisfactory results as shown in our empirical results presented in Table 2 and Appendix A.8. This inadequacy stems from the fact that the original input graph data (including node features) may not reside near a low-dimensional manifold (Bruna et al., 2013), while meaningful DMD-based stability analysis requires both the input and output data samples to lie near low-dimensional manifolds (Cheng et al., 2021). Therefore, a naive application of DMD metrics on the original graph structure is insufficient for assessing the stability of GNNs.

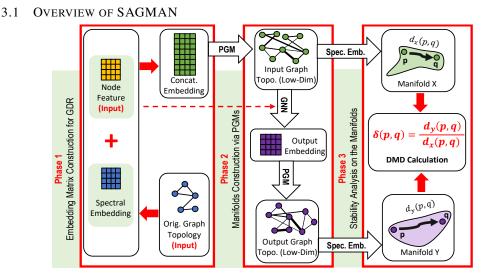


Figure 1: The proposed SAGMAN framework for stability analysis of GNNs on the manifolds.

To extend the applicability of the DMD metric to GNN settings, we introduce SAGMAN, a spectral framework for stability analysis of GNNs. A key component of SAGMAN is a novel distance-preserving Graph Dimensionality Reduction (GDR) algorithm that transforms the original input graph data—including node features and graph topology, which may reside in high-dimensional space—into a low-dimensional graph-based manifold.

As illustrated in Figure 1, the SAGMAN framework comprises three main phases:

- **Phase 1**: Creation of the input graph embedding matrix based on both node features and spectral properties of the graph. This embedding matrix is essential for the subsequent GDR step.
- **Phase 2**: Construction of low-dimensional input and output graph-based manifolds using a Probabilistic Graphical Model (PGM) approach.
- **Phase 3**: Node stability evaluation using the DMD metric, leveraging a spectral graph embedding scheme that utilizes generalized Laplacian eigenvalues and eigenvectors.
- 161 Detailed descriptions of each phase are provided in the following sections. The complete algorithmic flow of SAGMAN is shown in Section 3.5.

162 3.2 PHASE 1: EMBEDDING MATRIX CONSTRUCTION FOR GDR 163

164 The calculation of the DMD metric inherently relies on pairwise distances between nodes. For graph-based manifolds, two widely used metrics for evaluating pairwise node distances are: (1) the 165 shortest-path distance and (2) the effective resistance distance. As discussed in Appendix A.1, the 166 effective resistance distance is more closely related to the graph's structural (spectral) properties, 167 providing a more meaningful measure of connectivity between nodes. Moreover, previous studies 168 have demonstrated a significant correlation between effective resistance distances and the stability of machine learning models (Cheng et al., 2021). Therefore, our focus is on performing dimensionality 170 reduction on the input graph while preserving its original effective resistance distances. 171

172

Graph Dimensionality Reduction via Laplacian Eigenmaps. To achieve dimensionality reduction 173 of the input graph, we utilize the widely recognized nonlinear dimensionality reduction algorithm, 174 Laplacian Eigenmaps (Belkin & Niyogi, 2003). The Laplacian Eigenmaps algorithm begins by 175 constructing an undirected graph where each node represents a high-dimensional data sample, and 176 edges encode the similarities between data samples. It then computes the eigenvectors corresponding to the smallest eigenvalues of the graph Laplacian matrix, which are used to map each node into a 177 low-dimensional space while preserving the local relationships between the data samples. 178

179

Spectral Embedding with Eigengaps. For a graph with N nodes, a straightforward approach to 180 apply Laplacian Eigenmaps is to compute an $N \times N$ spectral embedding matrix using the complete 181 set of graph Laplacian eigenvectors and eigenvalues (Ng et al., 2001), representing each node with 182 an N-dimensional vector. However, computing the full set of eigenvalues and eigenvectors is 183 computationally prohibitive for large graphs. 184

185 To address this issue, we leverage a theoretical result from spectral graph clustering (Peng et al., 2015). which shows that the existence of a significant gap between consecutive eigenvalues-known as an 186 eigengap—implies that the graph can be well represented in a lower-dimensional space. Specifically, 187 the eigengap is defined as $\Upsilon(k) = \frac{\lambda_{k+1}}{\rho(k)}$, where $\rho(k)$ denotes the k-way expansion constant, and 188 189 λ_{k+1} is the (k+1)-th smallest eigenvalue of the normalized Laplacian matrix. A significant eigengap indicates the existence of a k-way partition where each cluster has low conductance, meaning the 190 graph is well-clustered. Based on this, we can approximate the spectral embedding using only the 191 first k eigenvalues and eigenvectors. We define the weighted spectral embedding matrix as follows: 192 **Definition 3.1.** For a connected graph G = (V, E, w) with its k smallest nonzero Laplacian eigen-193 values denoted by $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_k$ and corresponding eigenvectors u_1, u_2, \ldots, u_k , the 194 weighted spectral embedding matrix is defined as $U_k = \left[\frac{u_1}{\sqrt{\lambda_1}}, \dots, \frac{u_k}{\sqrt{\lambda_k}}\right] \in \mathbb{R}^{|V| \times k}$. 195

196

201

197 For a graph with a significant eigengap $\Upsilon(k)$, this embedding matrix allows us to represent each node with a k-dimensional vector such that the effective resistance distance between any pair of nodes can be well approximated by $d^{\text{eff}}(p,q) \approx \|U_k^\top e_{p,q}\|_2^2$, where $e_p \in \mathbb{R}^{|V|}$ is the standard basis vector with a 1 at position p and zeros elsewhere, and $e_{p,q} = e_p - e_q$. 199 200

- Using Eigengaps for Graph Dimension Estimation. Determining the precise graph dimension 202 required to embed a graph into Euclidean space while preserving certain properties (e.g., unit edge 203 lengths) is an NP-hard problem (Erdös et al., 1965; Schaefer, 2012). However, the presence of 204 a significant eigengap $\Upsilon(k)$ suggests that the graph can be well represented in a k-dimensional 205 space (Peng et al., 2015), making k an approximate measure of the graph's intrinsic dimensionality. 206 While computing the exact value of $\Upsilon(k)$ may be challenging in practice, we can use the identified 207 eigengap as an indicator of the suitability of SAGMAN for a given graph: graphs with significant 208 eigengaps are more suitable to our framework since they can be effectively represented in low-209 dimensional spaces. Empirically, for datasets with c classes, we can approximate k as $k \approx 10c$ to 210 effectively capture significant eigengaps (Deng et al., 2022).
- 211

212 3.3 PHASE 2: MANIFOLD CONSTRUCTION VIA PGMS

213

214 The embedding matrix U_k , derived in Phase 1 as defined in Definition 3.1, serves as the foundation for graph-based manifold construction in Phase 2. While the original Laplacian Eigenmaps algorithm 215

suggests constructing graph-based manifolds using k-nearest-neighbor graphs, we find that these

manifolds do not adequately preserve the original effective resistance distances. Consequently, they
 are not suitable for GNN stability analysis, as empirically demonstrated in Appendix A.6.

Probabilistic Graphical Models (PGMs) for Graph-based Manifold Learning. PGMs, also
 known as Markov Random Fields (MRFs), are powerful tools in machine learning and statistical
 physics for representing complex systems with intricate dependency structures (Roy et al., 2009).
 PGMs encode the conditional dependencies between random variables through an undirected graph
 structure (see Appendix A.3 for more details). Recent studies have shown that the graph structure
 learned through PGMs can have resistance distances that encode the Euclidean distances between
 their corresponding data samples (Feng, 2021).

In our context, each column vector in the embedding matrix U_k (as defined in Definition 3.1) corresponds to a data sample used for graph topology learning. By constructing the low-dimensional graph-based manifold via PGMs, we can effectively preserve the resistance distances from the original graph. Empirical evidence, detailed in Appendix A.6, supports that preserving these distances is essential for distinguishing between stable and unstable nodes. Therefore, our methodology leverages PGMs to maintain accurate effective resistance distances.

However, existing methods for learning PGMs may require numerous iterations to achieve convergence (Feng, 2021), limiting their applicability to large graphs.

Scalable PGM via Spectral Sparsification. In the proposed SAGMAN framework, we employ PGMs to create low-dimensional input graph-based manifold $G_X = (V, E_X)$ using the embedding matrix U_k from Definition 3.1, and output manifold $G_Y = (V, E_Y)$ using the GNN's post-*softmax* vectors, as illustrated in Figure 1. Below, we detail the construction of the input manifold; the output manifold can be constructed similarly. Given the input embedding matrix $X = U_k \in \mathbb{R}^{|V| \times k}$, the maximum likelihood estimation (MLE) of the precision matrix Θ (PGM) can be obtained by solving the following convex optimization problem (see Appendix A.3 for more details) (Dong et al., 2019):

$$\max_{\Theta} \quad F(\Theta) = \log \det(\Theta) - \frac{1}{k} \operatorname{Tr}(X^{\top} \Theta X),$$
(2)

243 244 245

252

253

258 259

260

242

where $\Theta = \mathcal{L} + \frac{1}{\sigma^2}I$, Tr(·) denotes the trace of a matrix, \mathcal{L} is a valid Laplacian matrix, I is the identity matrix, and $\sigma^2 > 0$ is a prior feature variance. To solve this, we give the following theorem:

Theorem 3.2. Maximizing the objective function in Equation 2 can be achieved in nearly-linear time via the following edge pruning strategy equivalent to spectral sparsification of the initial dense nearest-neighbor graph. Specifically, edges with small distance ratios

$$\rho_{p,q} = \frac{d^{\text{eff}}(p,q)}{d^{\text{dat}}(p,q)} = w_{p,q} d^{\text{eff}}(p,q)$$

are pruned, where $d^{\text{eff}}(p,q)$ is the effective resistance distance between nodes p and q, $d^{\text{dat}}(p,q) = \|X_p - X_q\|_2^2$ is the data distance between the embeddings of nodes p and q, and $w_{p,q} = \frac{1}{d^{\text{dat}}(p,q)}$ is the weight of edge (p,q).

The proof for Theorem 3.2 is available in Appendix A.4.

261 Spectral Sparsification via Graph Decomposition. Computing the edge sampling probability 262 $\rho_{p,q}$ for each edge (p,q) requires solving Laplacian matrices multiple times (Spielman & Srivastava, 263 2008), making the original sparsification method computationally expensive for large graphs. An 264 alternative approach employs a short-cycle graph decomposition scheme (Chu et al., 2020), which 265 partitions an unweighted graph *G* into multiple disjoint cycles by removing a fixed number of edges 266 while ensuring a bound on the length of each cycle. However, such methods are limited to unweighted 267 graphs.

Lemma 3.3. Spectral sparsification of an undirected graph G, with Laplacian L_G , can be achieved by leveraging a short-cycle decomposition algorithm that returns a sparsified graph H, with Laplacian L_H , such that for all real vectors x, $x^{\top}L_Gx \approx x^{\top}L_Hx$ (Chu et al., 2020). To extend these methods to weighted graphs, we introduce an improved spectral sparsification algorithm, illustrated in Figure 2. Our approach utilizes a *low-resistance-diameter* (LRD) decomposition scheme to limit the length of each cycle as measured by the effective resistance metric. This method is particularly effective for sparsifying weighted graphs.

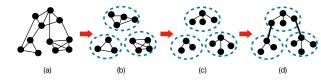


Figure 2: The proposed spectral sparsification algorithm. (a) The initial graph. (b) LRD decomposition for graph clustering. (c) LSSTs for pruning non-critical edges within clusters. (d) The final graph-based manifold with two inter-cluster edges.

The key idea is to efficiently compute the effective resistance of each edge (see Appendix A.9 for details) and employ a multilevel framework to decompose the graph into several disjoint clusters bounded by an effective resistance threshold. Importantly, the inter-cluster edges identified during this process can be inserted back into the original graph to significantly enhance the stability of GNN models, as demonstrated in Section 4.5.

3.4 PHASE 3: STABILITY ANALYSIS ON THE MANIFOLDS

δ

In this phase, we analyze the stability of GNNs by quantifying the distortions between the input and output graph-based manifolds constructed in Phase 2, utilizing the Distance Mapping Distortion (DMD) metric.

295 **DMD with Effective Resistance Distance Metric.** Let M be the mapping function of a machine learning model that transforms input data X into output data Y, i.e., Y = M(X). To assess the 296 stability of M, we employ the DMD metric, which measures how distances between data samples 297 are distorted by M. On the input and output graph-based manifolds, we use the *effective resistance* 298 *distance* as the metric between nodes. The effective resistance distance between nodes p and q on the 299 input manifold G_X is computed as $d_X^{\text{eff}}(p,q) = e_{p,q}^{\top} L_X^+ e_{p,q}$, and similarly on the output manifold 300 G_Y as $d_Y^{\text{eff}}(p,q) = e_{p,q}^{\top} L_Y^+ e_{p,q}$, where L_X^+ and L_Y^+ denote the Moore–Penrose pseudoinverses of the Laplacian matrices L_X and L_Y of the input and output manifolds, respectively, and $e_{p,q} = e_p - e_q$ 301 302 with e_p being the standard basis vector corresponding to node p. The DMD between nodes p and q is 303 defined as the ratio of the output distance to the input distance: 304

$${}^{M}(p,q) = \frac{d_{Y}^{\text{eff}}(p,q)}{d_{X}^{\text{eff}}(p,q)} = \frac{e_{p,q}^{\top} L_{Y}^{+} e_{p,q}}{e_{p,q}^{\top} L_{X}^{+} e_{p,q}}.$$
(3)

306 307 308

309

310

311

312 313

316

305

281

282 283

284

285

286

287

288 289

290

To quantify the maximum distortion introduced by M, we consider the maximum DMD over all pairs of distinct nodes: δ_{\max}^M . According to Lemma A.2 in (Cheng et al., 2021), the optimal Lipschitz constant K^* of the mapping M is bounded by the largest eigenvalue of $L_Y^+ L_X$ and the maximum DMD:

$$\delta_{\max}^{M} \le K^* \le \lambda_{\max}(L_Y^+ L_X). \tag{4}$$

This relationship allows us to assess the stability of M using spectral properties of the Laplacian matrices.

Node Stability Score via Spectral Embedding. Building on the theoretical insights from (Cheng et al., 2021), we utilize the largest generalized eigenvalues and their corresponding eigenvectors of $L_Y^+L_X$ to evaluate the stability of individual nodes in GNNs. We compute the weighted eigensubspace matrix $V_s \in \mathbb{R}^{|V| \times s}$ for spectral embedding of the input manifold $G_X = (V, E_X)$, where |V| is the number of nodes. The matrix V_s is defined as: $V_s = [v_1 \sqrt{\zeta_1}, v_2 \sqrt{\zeta_2}, \dots, v_s \sqrt{\zeta_s}]$, where $\zeta_1 \ge \zeta_2 \ge \dots \ge \zeta_s$ are the largest s eigenvalues of $L_Y^+L_X$, and v_1, v_2, \dots, v_s are the corresponding eigenvectors. Using V_s , we embed the nodes of G_X into an s-dimensional space by representing each node p with the p-th row of V_s . The stability of an edge $(p, q) \in E_X$ can then be estimated by 5

324 computing the spectral embedding distance between nodes p and q: $|V_s^{\top} e_{p,q}||_2^2$. To assess the stability 325 of individual nodes, we define the stability score of node p as the average embedding distance to its 326 neighbors in the input manifold: 327

328 329

331

333

335 336

337

365 366

$$score(p) = \frac{1}{|\mathbb{N}_X(p)|} \sum_{q \in \mathbb{N}_X(p)} \|V_s^{\top} e_{p,q}\|_2^2,$$
(5)

330 where $\mathbb{N}_X(p)$ denotes the set of neighbors of node p in G_X . Since $\|V_s^{\top} e_{p,q}\|_2^2$ is proportional to $(\delta^M(p,q))^3$, the node stability score effectively serves as a surrogate for the local Lipschitz constant, analogous to $\|\nabla_X M(p)\|$ under the manifold setting (Cheng et al., 2021). For a more detailed 332 derivation and theoretical justification, please refer to Appendix A.11. 334

3.5 Algorithm Flow of SAGMAN

The Algorithm 1 shows the key steps in SAGMAN.

aput: Graph $G = (V, E)$, node features X, GNN model autput: Stability scores for all nodes
1. Compute Spectral Embeddings (GDR):
• Compute the spectral embedding matrix U_k of G using its weighted Laplacian.
2. Augment Node Features:
• Concatenate X and U_k to form the feature matrix $FM = [U_k, X]$.
3. Construct Input Graph-based Manifold G_X (PGM):
• Build a k-NN graph G_{dense}^X using FM .
• Apply spectral sparsification to G_{dense}^X to obtain G_X .
4. Apply GNN Model:
• Compute output representations $Y = \text{GNN}(G_X, X)$.
5. Construct Output Graph-based Manifold G_Y (PGM):
• Build a k-NN graph G_{dense}^Y using Y.
• Apply spectral sparsification to G_{dense}^Y to obtain G_Y .
6. Compute Stability Scores (DMD):
• Compute Laplacians L_X and L_Y of G_X and G_Y .
• Solve the generalized eigenvalue problem $L_Y V_k = \lambda L_X V_k$ to obtain V_k .
• For each node $p \in V$:
- Compute the stability score: score $(p) = \frac{1}{ \mathcal{N}_X(p) } \sum_{q \in \mathcal{N}_X(p)} \ V_k^\top(e_p - e_q)\ _2^2$ wh
$\mathcal{N}_X(p)$ are the neighbors of p in G_X .

3.6 TIME COMPLEXITY OF SAGMAN

The proposed SAGMAN framework is designed to be efficient and scalable for large graphs. Below, 367 we analyze the time complexity of its key components. We utilize fast multilevel eigensolvers to 368 compute the first c Laplacian eigenvectors. These eigensolvers operate in nearly linear time, O(c|V|), 369 without loss of accuracy (Zhao et al., 2021), where |V| denotes the number of nodes in the graph. To 370 construct the initial graph for manifold learning, we employ the k-nearest neighbor algorithm, which 371 has a nearly linear computational complexity of $O(|V| \log |V|)$ (Malkov & Yashunin, 2018). The 372 spectral sparsification step, performed via Low-Resistance-Diameter (LRD) decomposition, has a 373 time complexity of O(|V|dm), where d is the average degree of the graph, and m is the order of the 374 Krylov subspace used in the computation. By leveraging fast generalized eigensolvers (Koutis et al., 375 2010; Cucuringu et al., 2016), we can compute all DMD values in O(|E|) time, where |E| denotes 376 the number of edges in the graph. Importantly, we ignore d (average degree) because most real-world graphs are sparse (Miao et al., 2019), with average degrees much smaller than the number of nodes. 377 In such cases, d can be treated as a constant or as growing slowly with |V|.

Overall, the dominant terms in the time complexity are nearly linear with respect to the size of the graph. This near-linear scalability allows SAGMAN to handle large graph datasets efficiently. Results for runtime scalability are available in Appendix A.13

4 EXPERIMENTS

We validate our proposed SAGMAN framework through comprehensive experiments. First, we compare exact resistance distances from the original graph with their approximations derived from the constructed manifold to demonstrate the manifold's fidelity. Next, we present numerical experiments showcasing the effectiveness of our metric in quantifying GNN stability. We then highlight the efficacy of our SAGMAN-guided approach in executing graph adversarial attacks. Finally, we demonstrate how leveraging the low-dimensional input manifold created by SAGMAN significantly enhances GNN stability. Details of our experimental setup are provided in Appendix A.5. We define a node as unstable if small perturbations in the input lead to significant changes in the output, indicated by a high DMD value. Conversely, a stable node has a low DMD value, reflecting robustness to input variations.

395 4.1 EVALUATION OF GRAPH DIMENSION REDUCTION (GDR)

A natural concern arises regarding how much the constructed input graph-based manifold might change the original graph's structure. To this end, we compare the exact resistance distances calculated using the complete set of eigenpairs with approximate resistance distances estimated using the embedding matrix U_k (as defined in Definition 3.1), considering various values of k as shown in Table 1. Our empirical results demonstrate that using a small number of eigenpairs can effectively approximate the original effective-resistance distances. Furthermore, Table 2 shows that the SAGMAN-guided stability analysis with GDR consistently distinguishes between stable and unstable nodes, whereas the analysis without GDR fails to do so. Additional related results for various datasets and GNN architectures are provided in Appendix A.8.

Table 1: Resistance-distance preservation for the Cora graph, evaluating 100 randomly selected node pairs. Larger correlation coefficients (CC) indicate more accurate estimations.

k	20	30	50	100	200	400	500
CC	0.69	0.78	0.82	0.87	0.93	0.97	0.99

Table 2: Cosine similarities between original and perturbed node embeddings for stable/unstable
 nodes under Nettack adversarial attacks on the Cora dataset using GCN. Higher cosine similarities
 for stable nodes and lower for unstable nodes indicate better distinction. Better results are in **bold**.

Nettack Level	1	2	3
w/o GDR	0.90/0.96	0.84/0.93	0.81/0.91
w/ GDR	0.99/0.90	0.98/0.84	0.97/0.81

Table 3: Comparison of Nettack/FGA error rates for 40 nodes selected using Nettack's recommen dation, confidence ranking, and SAGMAN. All nodes chosen by SAGMAN-guided methods are
 correctly classified before perturbation. Better results are highlighted in **bold**.

,		1	00	
1	Selection	Nettack's default	Confidence Ranking	SAGMAN
2	Cora	0.725/0.850	0.925/0.775	0.975/0.975
3	Cora-ml	0.750/0.850	0.800/0.700	0.950/0.950
1	Citeseer	0.800/0.875	0.925/0.950	1.000/0.975
5	Pubmed	0.750/0.875	0.750/0.925	0.825/0.950
-				

427 4.2 METRICS FOR GNN STABILITY EVALUATION

We empirically demonstrate SAGMAN's ability to distinguish between stable and unstable samples
under DICE attack (Waniek et al., 2018) and Gaussian perturbation, as shown in Figure 3. Additional results on PGD attack, various datasets—including large-scale datasets—and different GNN
architectures under Nettack attacks (Zügner et al., 2018) are provided in Appendix A.10, further
illustrating the effectiveness of our metric. SAGMAN is most effective for GNNs that perform feature

Table 4: Error rates for the Cora and Citeseer datasets before/after Nettack and IG-attack evasion attacks, with and without SAGMAN enhancement. 'Size' indicates the fraction of the nodes selected. Better results are highlighted in **bold**.

Nettack	Attack Budget Size	1%	5%	10%	15%	20%
Cora	w/o SAGMAN w/ SAGMAN	0.00/0.79 0.00/0.00	0.01/0.86 0.00/0.00	0.01/0.90 0.01/0.01	0.02 /0.93 0.06/ 0.06	0.02 /0.92 0.08/ 0.08
Citeseer	w/o SAGMAN w/ SAGMAN	0.00 /0.76 0.09/ 0.42	0.03 /0.82 0.10/ 0.37	0.04 /0.85 0.12/ 0.37	0.04 /0.86 0.11/ 0.35	0.03 /0.85 0.08/ 0.28
IG-attac	k Budget Size	1%	5%	10%	15%	20%
Citeseer	w/o SAGMAN w/ SAGMAN	0.00/0.76 0.00/0.05	0.02/0.74 0.02/0.07	0.02/0.74 0.02/0.07	0.02/0.72 0.02/0.04	0.02/0.75 0.02/0.09
Cora	w/o SAGMAN w/ SAGMAN	0.00/0.96 0.00/0.00	0.02/0.83 0.02/0.02	0.02/0.81 0.02/0.03	0.02/0.82 0.02/0.02	0.02/0.81 0.02/0.04

Table 5: Baseline and Perturbed error rates for the Citeseer dataset using GOOD-AT, SAGMAN, and both. Our experiments' attack method and backbone architecture follow those from Li et al. (2024). The best results are marked in **bold**, and the second-best results are underlined.

Edge Attack Budget	25	109	219	302	410	550
GCN(baseline)	0.2968	0.3211	0.3590	0.3780	0.4064	0.4301
GOOD-AT	0.2808	0.2820	0.2850	0.2838	0.2855	0.2915
SAGMAN	0.2808	0.2802	0.2808	0.2820	0.2814	0.2838
GOOD-AT+SAGMAN	0.2684	0.2695	0.2684	0.2690	0.2690	0.2701

smoothing, common in homophilic graphs. However, for heterophilic graphs, we still observed SAGMAN distinguish stable and unstable nodes, as shown in Figure 10

4.3 STABILITY OF GNN-BASED RECOMMENDATION SYSTEMS

We evaluate the stability of GNN-based recommendation systems using the PinSage framework (Ying et al., 2018) on the MovieLens 1M dataset (Harper & Konstan, 2015). To construct the input graph, we first homogenize the various node and edge types into a unified format. We then calculate the weighted spectral embedding matrix U_k (as defined in Definition 3.1) and extract user-type samples to build a low-dimensional input (user) graph-based manifold. For the output graph-based manifold, we utilize PinSage's final output, which includes the top-10 recommended items for each user. We construct this output (user) graph-based manifold based on Jaccard similarity measures of these recommendations. Table 6 demonstrates the effectiveness of SAGMAN in distinguishing between stable and unstable users.

Table 6: Comparison of the mean Jaccard similarity (MJS) between SAGMAN-selected stable/unstable users at a perturbation level (l) ranging from 1 to 5 where each selected user is connected to l randomly chosen new items. The MJS is computed over 20 iterations for each perturbation.

Perturbation Level	1	2	3	4	5
Stable Users	0.8513	0.8837	0.8295	0.8480	0.8473
Unstable Users	0.7885	0.7955	0.8167	0.8278	0.7794

SAGMAN-GUIDED ADVERSARIAL TARGETED ATTACK 4.4

We adapt our GNN training methodology from previous work (Jin et al., 2021). Using GCN as our base model for the Citeseer, Cora, Cora-ML, and Pubmed datasets, we employ Nettack and FGA (Chen et al., 2018) as benchmark attack methods. For target node selection, we compare NetClambelon.gprg/m Clambelon.gprg/m Clambelon.gp

Figure 3: The horizontal axes, denoted by X, represent the perturbation applied. 'Random EdgesPT' refers to the DICE attack. 'Random FeaturePT' indicates the application of Gaussian noise perturbation, expressed as $X\eta$ perturbation, where η represents Gaussian noise. SAGMAN Stable/Unstable denotes the samples classified as stable or unstable by SAGMAN, respectively.

tack's recommendation (Zügner et al., 2018), SAGMAN-guided strategies, and a heuristic confidence ranking (Chang et al., 2017).

Table 3 presents the error rates after applying Nettack and FGA attacks. The results demonstrate that SAGMAN-guided attacks outperform both Nettack's recommendation and the confidence ranking, leading to more effective adversarial attacks.

509 4.5 SAGMAN-GUIDED GNN STABILITY ENHANCEMENT

A naive approach to improving the stability of a GNN model is to replace the entire input graph with 511 the low-dimensional graph-based manifold for GNN predictions. However, due to the significantly 512 increased densities in the graph-based manifold, the GNN prediction accuracy may be adversely 513 affected. To achieve a flexible trade-off between model stability and prediction accuracy, we select 514 only the inter-cluster edges from the input graph-based manifold, as shown in Figure 2(d), and 515 insert them into the original graph. Since the inter-cluster (bridge-like) edges are typically spectrally 516 critical—with high sampling probabilities as defined in Theorem 3.2—adding them to the original 517 graph significantly alters its structural (spectral) properties. 518

Whereas previous work (Deng et al., 2022) focuses on improving the robustness of GNNs against 519 poisoning attacks, our work centers on enhancing robustness against evasion attacks. In Table 4, we 520 present the error rates for both the original and the enhanced graphs, where Nettack was employed to 521 perturb SAGMAN-selected most unstable samples within each graph. Table 5 shows the error rates for 522 the state-of-the-art GOOD-AT (Li et al., 2024) method and our proposed SAGMAN approach. Since 523 SAGMAN is a versatile plug-in method that can be combined with other robustness techniques, we 524 also report results for the combined application of GOOD-AT and SAGMAN. Notably, reintegrating selected edges into the original graph significantly reduces the error rate when subjected to adversarial 526 evasion attacks. To further demonstrate SAGMAN's effectiveness under poisoning attacks and in 527 comparison with Lipschitz-based methods, we present additional results in Appendix A.13.

528 529

498

499

500

501

508

510

5 CONCLUSIONS

530 531

In this work, we introduced SAGMAN, a novel framework for analyzing the stability of GNNs at
the individual node level by assessing the resistance-distance distortions between low-dimensional
input and output graph-based manifolds. A key component of SAGMAN is the proposed Graph
Dimensionality Reduction (GDR) approach for constructing resistance-preserving manifolds, which
enables effective stability analysis.

Our experimental results demonstrate that SAGMAN effectively quantifies GNN stability, leading to
 significantly enhanced targeted adversarial attacks and improved GNN robustness. The current SAG MAN framework is particularly effective for graphs that can be well represented in low-dimensional
 spaces and exhibit large eigengaps.

540 REFERENCES

565

566

570

571

572

- 542 Mikhail Belkin and Partha Niyogi. Laplacian eigenmaps for dimensionality reduction and data
 543 representation. *Neural computation*, 15(6):1373–1396, 2003.
- Aleksandar Bojchevski and Stephan Günnemann. Adversarial attacks on node embeddings via graph poisoning. In *International Conference on Machine Learning*, pp. 695–704. PMLR, 2019.
- Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral networks and locally
 connected networks on graphs. *arXiv preprint arXiv:1312.6203*, 2013.
- Haw-Shiuan Chang, Erik Learned-Miller, and Andrew McCallum. Active bias: Training more accurate neural networks by emphasizing high variance samples. *Advances in Neural Information Processing Systems*, 30, 2017.
- Jinyin Chen, Yangyang Wu, Xuanheng Xu, Yixian Chen, Haibin Zheng, and Qi Xuan. Fast gradient
 attack on network embedding. *arXiv preprint arXiv:1809.02797*, 2018.
- Wuxinlin Cheng, Chenhui Deng, Zhiqiang Zhao, Yaohui Cai, Zhiru Zhang, and Zhuo Feng. Spade:
 A spectral method for black-box adversarial robustness evaluation. In *International Conference on Machine Learning*, pp. 1814–1824. PMLR, 2021.
- Eli Chien, Jianhao Peng, Pan Li, and Olgica Milenkovic. Adaptive universal generalized pagerank
 graph neural network. *arXiv preprint arXiv:2006.07988*, 2020.
- Timothy Chu, Yu Gao, Richard Peng, Sushant Sachdeva, Saurabh Sawlani, and Junxing Wang. Graph sparsification, spectral sketches, and faster resistance computation via short cycle decompositions. *SIAM Journal on Computing*, (0):FOCS18–85, 2020.
 - Fan RK Chung. Spectral graph theory, volume 92. American Mathematical Soc., 1997.
- Mihai Cucuringu, Ioannis Koutis, Sanjay Chawla, Gary Miller, and Richard Peng. Simple and
 scalable constrained clustering: a generalized spectral method. In *Artificial Intelligence and Statistics*, pp. 445–454. PMLR, 2016.
 - Enyan Dai, Tianxiang Zhao, Huaisheng Zhu, Junjie Xu, Zhimeng Guo, Hui Liu, Jiliang Tang, and Suhang Wang. A comprehensive survey on trustworthy graph neural networks: Privacy, robustness, fairness, and explainability. *Machine Intelligence Research*, pp. 1–51, 2024.
- 574 Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on
 575 graphs with fast localized spectral filtering. *Advances in neural information processing systems*,
 576 29, 2016.
- 577
 578
 578
 579
 Chenhui Deng, Xiuyu Li, Zhuo Feng, and Zhiru Zhang. Garnet: Reduced-rank topology learning for robust and scalable graph neural networks. *arXiv preprint arXiv:2201.12741*, 2022.
- Chenhui Deng, Zichao Yue, and Zhiru Zhang. Polynormer: Polynomial-expressive graph transformer
 in linear time. *arXiv preprint arXiv:2403.01232*, 2024.
- Xiaowen Dong, Dorina Thanou, Michael Rabbat, and Pascal Frossard. Learning graphs from data: A signal representation perspective. *IEEE Signal Processing Magazine*, 36(3):44–63, 2019.
- Paul Erdös, Frank Harary, and William T Tutte. On the dimension of a graph. *Mathematika*, 12(2):
 118–122, 1965.
- Wenqi Fan, Yao Ma, Qing Li, Yuan He, Eric Zhao, Jiliang Tang, and Dawei Yin. Graph neural networks for social recommendation. In *The world wide web conference*, pp. 417–426, 2019.
- Zhuo Feng. Sgl: Spectral graph learning from measurements. In 2021 58th ACM/IEEE Design Automation Conference (DAC), pp. 727–732. IEEE, 2021.
- Jerome Friedman, Trevor Hastie, and Robert Tibshirani. Sparse inverse covariance estimation with the graphical lasso. *Biostatistics*, 9(3):432–441, 2008.

594 595 596	Fernando Gama, Joan Bruna, and Alejandro Ribeiro. Stability properties of graph neural networks. <i>IEEE Transactions on Signal Processing</i> , 68:5680–5695, 2020.
597 598	Johannes Gasteiger, Aleksandar Bojchevski, and Stephan Günnemann. Predict then propagate: Graph neural networks meet personalized pagerank. <i>arXiv preprint arXiv:1810.05997</i> , 2018.
599 600	Gene H Golub and Charles F Van Loan. Matrix computations, volume 3. JHU press, 2013.
601 602	Alessio Gravina, Davide Bacciu, and Claudio Gallicchio. Anti-symmetric dgn: a stable architecture for deep graph networks. <i>arXiv preprint arXiv:2210.09789</i> , 2022.
603 604 605 606	Aditya Grover and Jure Leskovec. node2vec: Scalable feature learning for networks. In <i>Proceedings</i> of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pp. 855–864, 2016.
607 608	F Maxwell Harper and Joseph A Konstan. The movielens datasets: History and context. Acm transactions on interactive intelligent systems (tiis), 5(4):1–19, 2015.
609 610 611 612	Ziniu Hu, Yuxiao Dong, Kuansan Wang, Kai-Wei Chang, and Yizhou Sun. Gpt-gnn: Generative pre-training of graph neural networks. In <i>Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining</i> , pp. 1857–1867, 2020.
613 614 615	Weizhe Hua, Yichi Zhang, Chuan Guo, Zhiru Zhang, and G Edward Suh. Bullettrain: Accelerating robust neural network training via boundary example mining. <i>Advances in Neural Information Processing Systems</i> , 34:18527–18538, 2021.
616 617 618 619	Yinan Huang, William Lu, Joshua Robinson, Yu Yang, Muhan Zhang, Stefanie Jegelka, and Pan Li. On the stability of expressive positional encodings for graph neural networks. <i>arXiv preprint arXiv:2310.02579</i> , 2023.
620 621 622	Yaning Jia, Dongmian Zou, Hongfei Wang, and Hai Jin. Enhancing node-level adversarial defenses by lipschitz regularization of graph neural networks. In <i>Proceedings of the 29th ACM SIGKDD</i> <i>Conference on Knowledge Discovery and Data Mining</i> , pp. 951–963, 2023.
623 624	Wei Jin, Yaxin Li, Han Xu, Yiqi Wang, and Jiliang Tang. Adversarial attacks and defenses on graphs: A review and empirical study. <i>arXiv preprint arXiv:2003.00653</i> , 10(3447556.3447566), 2020.
625 626 627	Wei Jin, Yaxing Li, Han Xu, Yiqi Wang, Shuiwang Ji, Charu Aggarwal, and Jiliang Tang. Adversarial attacks and defenses on graphs. <i>ACM SIGKDD Explorations Newsletter</i> , 22(2):19–34, 2021.
628 629	Vassilis Kalofolias and Nathanaël Perraudin. Large scale graph learning from smooth signals. International Conference on Learning Representations (ICLR 2019), 2019.
630 631 632	Ryan Keisler. Forecasting global weather with graph neural networks. <i>arXiv preprint arXiv:2202.07575</i> , 2022.
633 634 635	Henry Kenlay, Dorina Thanou, and Xiaowen Dong. Interpretable stability bounds for spectral graph filters. In <i>International conference on machine learning</i> , pp. 5388–5397. PMLR, 2021.
636 637 638	Nicolas Keriven, Alberto Bietti, and Samuel Vaiter. Convergence and stability of graph convolutional networks on large random graphs. <i>Advances in Neural Information Processing Systems</i> , 33: 21512–21523, 2020.
639 640 641	Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. <i>arXiv preprint arXiv:1609.02907</i> , 2016.
642 643	Douglas J Klein and H-Y Zhu. Distances and volumina for graphs. <i>Journal of mathematical chemistry</i> , 23(1):179–195, 1998.
644 645 646 647	Ioannis Koutis, Gary L Miller, and Richard Peng. Approaching optimality for solving sdd linear systems. In <i>Foundations of Computer Science (FOCS), 2010 51st Annual IEEE Symposium on</i> , pp. 235–244. IEEE, 2010.

Brenden Lake and Joshua Tenenbaum. Discovering structure by learning sparse graphs. 2010.

648 649	John M Lee. Smooth manifolds. Springer, 2012.
650 651 652	Kuan Li, YiWen Chen, Yang Liu, Jin Wang, Qing He, Minhao Cheng, and Xiang Ao. Boosting the adversarial robustness of graph neural networks: An ood perspective. In <i>The Twelfth International Conference on Learning Representations</i> , 2024.
653 654 655 656	Yu A Malkov and Dmitry A Yashunin. Efficient and robust approximate nearest neighbor search using hierarchical navigable small world graphs. <i>IEEE transactions on pattern analysis and machine intelligence</i> , 42(4):824–836, 2018.
657 658	Jianyu Miao, Tiejun Yang, Junwei Jin, and Lingfeng Niu. Graph-based clustering via group sparsity and manifold regularization. <i>IEEE Access</i> , 7:172123–172135, 2019.
659 660 661 662	Azalia Mirhoseini, Anna Goldie, Mustafa Yazgan, Joe Wenjie Jiang, Ebrahim Songhori, Shen Wang, Young-Joon Lee, Eric Johnson, Omkar Pathak, Azade Nazi, et al. A graph placement methodology for fast chip design. <i>Nature</i> , 594(7862):207–212, 2021.
663 664	Andrew Ng, Michael Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. <i>Advances in neural information processing systems</i> , 14, 2001.
665 666 667	Sinno Jialin Pan and Qiang Yang. A survey on transfer learning. <i>IEEE Transactions on knowledge and data engineering</i> , 22(10):1345–1359, 2009.
668 669	Richard Peng, He Sun, and Luca Zanetti. Partitioning well-clustered graphs: Spectral clustering works! In <i>Conference on learning theory</i> , pp. 1423–1455. PMLR, 2015.
670 671 672	Édgar Roldán and Juan MR Parrondo. Entropy production and kullback-leibler divergence between stationary trajectories of discrete systems. <i>Physical Review E</i> , 85(3):031129, 2012.
673 674 675	Sushmita Roy, Terran Lane, and Margaret Werner-Washburne. Learning structurally consistent undirected probabilistic graphical models. In <i>Proceedings of the 26th annual international conference on machine learning</i> , pp. 905–912, 2009.
676 677 678	Marcus Schaefer. Realizability of graphs and linkages. In <i>Thirty Essays on Geometric Graph Theory</i> , pp. 461–482. Springer, 2012.
679 680 681	Kartik Sharma, Samidha Verma, Sourav Medya, Arnab Bhattacharya, and Sayan Ranu. Task and model agnostic adversarial attack on graph neural networks. In <i>Proceedings of the AAAI Conference on Artificial Intelligence</i> , volume 37, pp. 15091–15099, 2023.
682 683 684 685	Martin Slawski and Matthias Hein. Estimation of positive definite m-matrices and structure learning for attractive gaussian markov random fields. <i>Linear Algebra and its Applications</i> , 473:145–179, 2015.
686 687 688	Yang Song, Qiyu Kang, Sijie Wang, Kai Zhao, and Wee Peng Tay. On the robustness of graph neural diffusion to topology perturbations. <i>Advances in Neural Information Processing Systems</i> , 35: 6384–6396, 2022.
689 690 691	Daniel A Spielman and Nikhil Srivastava. Graph sparsification by effective resistances. In <i>Proceedings</i> of the fortieth annual ACM symposium on Theory of computing, pp. 563–568, 2008.
692 693	Daniel A Spielman and Shang-Hua Teng. Spectral sparsification of graphs. <i>SIAM Journal on Computing</i> , 40(4):981–1025, 2011.
694 695 696 697	Yiwei Sun, Suhang Wang, Xianfeng Tang, Tsung-Yu Hsieh, and Vasant Honavar. Adversarial attacks on graph neural networks via node injections: A hierarchical reinforcement learning approach. In <i>Proceedings of the Web Conference 2020</i> , pp. 673–683, 2020.
698 699	Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, and Rob Fergus. Intriguing properties of neural networks. <i>arXiv preprint arXiv:1312.6199</i> , 2013.
700 701	Joshua B Tenenbaum, Vin de Silva, and John C Langford. A global geometric framework for nonlinear dimensionality reduction. <i>science</i> , 290(5500):2319–2323, 2000.

- Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.
- Marcin Waniek, Tomasz P Michalak, Michael J Wooldridge, and Talal Rahwan. Hiding individuals
 and communities in a social network. *Nature Human Behaviour*, 2(2):139–147, 2018.
- Qitian Wu, Chenxiao Yang, Wentao Zhao, Yixuan He, David Wipf, and Junchi Yan. Difformer: Scalable (graph) transformers induced by energy constrained diffusion. *arXiv preprint arXiv:2301.09474*, 2023.
- Kaidi Xu, Hongge Chen, Sijia Liu, Pin-Yu Chen, Tsui-Wei Weng, Mingyi Hong, and Xue Lin.
 Topology attack and defense for graph neural networks: An optimization perspective. *arXiv* preprint arXiv:1906.04214, 2019.
- Liang Yao, Chengsheng Mao, and Yuan Luo. Graph convolutional networks for text classification. In Proceedings of the AAAI conference on artificial intelligence, volume 33, pp. 7370–7377, 2019.
- Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L Hamilton, and Jure Leskovec.
 Graph convolutional neural networks for web-scale recommender systems. In *Proceedings of the* 24th ACM SIGKDD international conference on knowledge discovery & data mining, pp. 974–983, 2018.
- Bing Yu, Haoteng Yin, and Zhanxing Zhu. Spatio-temporal graph convolutional networks: A deep learning framework for traffic forecasting. *arXiv preprint arXiv:1709.04875*, 2017.
- Kai Zhao, Qiyu Kang, Yang Song, Rui She, Sijie Wang, and Wee Peng Tay. Adversarial robustness in graph neural networks: A hamiltonian approach. *Advances in Neural Information Processing Systems*, 36, 2024.
- Zhiqiang Zhao, Ying Zhang, and Zhuo Feng. Towards scalable spectral embedding and data visual ization via spectral coarsening. In *Proceedings of the 14th ACM International Conference on Web Search and Data Mining*, pp. 869–877, 2021.
- Jie Zhou, Ganqu Cui, Shengding Hu, Zhengyan Zhang, Cheng Yang, Zhiyuan Liu, Lifeng Wang,
 Changcheng Li, and Maosong Sun. Graph neural networks: A review of methods and applications.
 AI open, 1:57–81, 2020.
 - Dingyuan Zhu, Ziwei Zhang, Peng Cui, and Wenwu Zhu. Robust graph convolutional networks against adversarial attacks. In *Proceedings of the 25th ACM SIGKDD international conference on knowledge discovery & data mining*, pp. 1399–1407, 2019.
 - Daniel Zügner, Amir Akbarnejad, and Stephan Günnemann. Adversarial attacks on neural networks for graph data. In *Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining*, pp. 2847–2856, 2018.
- 743 744 745

707

722

732

736

737

738

739 740

741

742

- A APPENDIX
- 746 747
- 111121021
- A.1 GRAPH-BASED MANIFOLDS AND DISTANCE METRICS

Graph-based Manifolds. A manifold is a topological space that locally resembles Euclidean space near each point (Lee, 2012). In our work, we utilize *graph-based manifolds* to represent complex data structures. Specifically, we represent each manifold as an undirected (connected) graph G = (V, E), where V is the set of vertices corresponding to data points, and E is the set of edges encoding relationships (e.g., conditional dependencies) between these points (Tenenbaum et al., 2000). This representation is particularly effective when the underlying data structure can be approximated by a network of discrete points, as is common in spectral clustering and manifold learning (Belkin & Niyogi, 2003). ⁷⁵⁶ **Mappings Between Manifolds.** Understanding the *mappings between manifolds* is essential for ⁷⁵⁷ transferring and comparing information across different data representations. In our context, these ⁷⁵⁸ mappings correspond to transformations between the input and output graph-based manifolds of ⁷⁵⁹ an ML model. Formally, a mapping $\varphi : M_X \to M_Y$ from the input manifold M_X to the output ⁷⁶⁰ manifold M_Y allows us to analyze how the model transforms data points and their relationships (Pan ⁷⁶¹ & Yang, 2009). This is crucial for assessing the model's stability with respect to small perturbations ⁷⁶² in the input.

763

Distance Metrics on Manifolds. Measuring dissimilarities between points on manifolds requires appropriate distance metrics. While *geodesic distances*, representing the shortest paths between points on a manifold, are commonly used, they can be computationally intensive for large datasets and may not capture global structural information due to their inherently local nature (Tenenbaum et al., 2000).

769

Fifective Resistance Distances on Graph-based Manifolds. To overcome these limitations, we employ the *effective resistance distance* from electrical network theory. By modeling the undirected graph as a resistive network, the effective resistance between two nodes captures both local relation-ships and global structural properties of the graph. This metric effectively combines the advantages of geodesic and global distances, providing a more comprehensive measure of similarity in graph-based manifolds (Tenenbaum et al., 2000). Additionally, it is computationally efficient for large-scale graphs (Klein & Zhu, 1998), making it practical for our analysis.

To illustrate the difference between geodesic distance and effective resistance distance, consider the example in Figure 4. In all three graphs, nodes A and B have the same geodesic distance (i.e., the shortest path length is identical). However, their effective resistance distances Ω_{AB} vary significantly due to differences in the global structure of each graph. This example demonstrates that while geodesic distance only accounts for the shortest path, effective resistance distance incorporates the overall connectivity and network topology, making it a more informative metric for assessing similarities in graph-based manifolds.

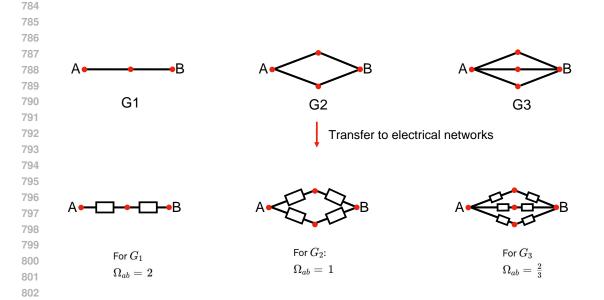


Figure 4: Examples of three different graph structures with nodes A and B. Despite having the same geodesic distance (shortest path length), the effective resistance distances Ω_{AB} vary due to the different global structures of the graphs.

807

803

By incorporating effective resistance distances into our stability analysis, we can more accurately
 assess the distance distortions introduced by the mappings between the input and output manifolds (as discussed in Section 2.1). This provides a solid foundation for evaluating the stability of ML

810 models on graph-based manifolds, enhancing both the theoretical rigor and practical applicability of 811 our approach. 812

813 A.2 SPECTRAL GRAPH THEORY 814

815 Spectral graph theory is a branch of mathematics that studies the properties of graphs through the 816 eigenvalues and eigenvectors of matrices associated with the graph (Chung, 1997). Let G = (V, E, w)denote an undirected graph G, V denote a set of nodes (vertices), E denote a set of edges and w817 818 denote the corresponding edge weights. The adjacency matrix can be defined as:

$$A(i,j) = \begin{cases} w(i,j) & \text{if } (i,j) \in E\\ 0 & \text{otherwise} \end{cases}$$
(6)

The Laplacian matrix of G can be constructed by L = D - A, where D denotes the degree matrix. Lemma A.1. (Courant-Fischer Minimax Theorem) The k-th largest eigenvalue of the Laplacian matrix $L \in \mathbb{R}^{|V| \times |V|}$ can be computed as follows:

$$\lambda_k(L) = \min_{\substack{\dim(U)=k \\ u_k \neq 0}} \max_{\substack{u_k \in U \\ u_k \neq 0}} \frac{u_k^{\top} L u_k}{u_k^{\top} u_k}$$
(7)

829 Lemma A.1 is the Courant-Fischer Minimax Theorem (Golub & Van Loan, 2013) for solving the 830 eigenvalue problem: $Lu_k = \lambda_k u_k$. The generalized Courant-Fischer Minimax Theorem for solving 831 generalized eigenvalue problem $L_X v_k = \lambda_k L_Y v_k$ can be expressed as follows:

832 Lemma A.2. (The Generalized Courant-Fischer Minimax Theorem) Given two Laplacian matri-833 ces $L_X, L_Y \in \mathbb{R}^{|V| \times |V|}$ such that $null(L_Y) \subseteq null(L_X)$, L_Y^+ denotes the Moore–Penrose pseu-834 doinverse of L_Y , the k-th largest eigenvalue of $L_Y^+L_X$ can be computed under the condition of 835 $1 \leq k \leq rank(L_Y)$ by: 836

$$\lambda_k(L_Y^+ L_X) = \min_{\substack{\dim(U)=k\\U\perp null(L_Y)}} \max_{v_k \in U} \frac{v_k^+ L_X v_k}{v_k^\top L_Y v_k}.$$
(8)

838 839 840

841

845

837

823

824

825 826 827

828

A.3 **GRAPH-BASED MANIFOLD LEARNING VIA PGMS**

842 Given M samples of N-dimensional vectors stored in a data matrix $X \in \mathbb{R}^{N \times M}$, the recent 843 graph topology learning methods (Kalofolias & Perraudin, 2019; Dong et al., 2019) estimate graph 844 Laplacians from X for achieving the following desired characteristics:

Smoothness of Graph Signals. The graph signals corresponding to the real-world data should be 846 sufficiently smooth on the learned graph structure: the signal values will only change gradually across 847 connected neighboring nodes. The smoothness of a signal x over an undirected graph G = (V, E, w)848 can be measured with the following Laplacian quadratic form: $x^{\top}Lx = \sum w_{p,q}(x(p) - x(q))^2$, 849 $(p,q) \in E$

850 where $w_{p,q}$ denotes the weight of edge (p,q), L = D - W denotes the Laplacian, D denotes the diagonal (degree) matrix, and W denotes the adjacency matrix of G, respectively. The smaller 851 quadratic form implies the smoother signals across the edges in the graph. The smoothness (Q) of 852 a set of signals X over graph G is computed using the following matrix trace (Dong et al., 2019): 853 $Q(X,L) = Tr(X^{\top}LX)$, where $Tr(\bullet)$ denotes the matrix trace. 854

855 **Sparsity of the Estimated Graph.** Graph sparsity is another critical consideration in graph learning. 856 One of the most important motivations of learning a graph is to use it for downstream computing tasks. Therefore, more desired graph topology learning algorithms should allow better capturing and understanding the global structure (manifold) of the data set, while producing sufficiently sparse 858 graphs that can be easily stored and efficiently manipulated in the downstream algorithms, such as 859 circuit simulations, network partitioning, dimensionality reduction, data visualization, etc. 860

861 **Problem Formulation.** Consider a random vector $x \sim N(0, \Sigma)$ with probability density function: 862

/ A -

$$f(x) = \frac{\exp\left(-\frac{1}{2}x^{\top}\Sigma^{-1}x\right)}{(2\pi)^{N/2}\det(\Sigma)^{(1/2)}} \propto \det(\Theta)^{1/2}\exp\left(-\frac{1}{2}x^{\top}\Theta x\right),\tag{9}$$

where $\Sigma = \mathbb{E}[xx^{\top}] \succ 0$ denotes the covariance matrix, and $\Theta = \Sigma^{-1}$ denotes the precision matrix (inverse covariance matrix). Prior graph topology learning methods aim at estimating sparse precision matrix Θ from potentially high-dimensional input data, which fall into the following two categories:

(A) The graphical Lasso method aims at estimating a sparse precision matrix Θ using convex optimization to maximize the log-likelihood of f(x) (Friedman et al., 2008):

$$\max_{\Theta} : \log \det(\Theta) - Tr(\Theta S) - \beta \|\Theta\|_1, \tag{10}$$

872 where Θ denotes a non-negative definite precision matrix, S denotes a sample covariance matrix, 873 and β denotes a regularization parameter. The first two terms together can be interpreted as the 874 log-likelihood under a Gaussian Markov Random Field (GMRF). $\|\bullet\|$ denotes the entry-wise ℓ_1 norm, 875 so $\beta \|\Theta\|_1$ becomes the sparsity promoting regularization term. This model learns the graph structure 876 by maximizing the penalized log-likelihood. When the sample covariance matrix S is obtained from 877 M i.i.d (independent and identically distributed) samples $X = [x_1, ..., x_M]$ where $X \sim N(0, S)$ has an N-dimensional Gaussian distribution with zero mean, each element in the precision matrix $\Theta_{i,i}$ 878 encodes the conditional dependence between variables X_i and X_j . For example, $\Theta_{i,j} = 0$ implies 879 that variables X_i and X_j are conditionally independent, given the rest. 880

(B) The Laplacian estimation methods have been recently introduced for more efficiently solving
 the following convex problem (Dong et al., 2019; Lake & Tenenbaum, 2010):

$$\max_{\Theta} : F(\Theta) = \log \det(\Theta) - \frac{1}{M} Tr(X^{\top} \Theta X) - \beta \|\Theta\|_{1},$$
(11)

886 where $\Theta = L + \frac{1}{\sigma^2}I$, L denotes the set of valid graph Laplacian matrices, I denotes the identity 887 matrix, and $\sigma^2 > 0$ denotes prior feature variance. It can be shown that the three terms in (11) are 888 corresponding to $\log \det(\Theta)$, $Tr(\Theta S)$ and $\beta \|\Theta\|_1$ in (10), respectively. Note that the second term 889 also promotes graph sparsity, so the $\beta \|\Theta\|_1$ can be dropped without impacting the final solution. Since 890 $\Theta = L + \frac{1}{r^2}I$ correspond to symmetric and positive definite (PSD) matrices (or M matrices) with 891 non-positive off-diagonal entries, this formulation will lead to the estimation of attractive GMRFs 892 (Dong et al., 2019; Slawski & Hein, 2015). In case X is non-Gaussian, formulation (11) can be 893 understood as Laplacian estimation based on minimizing the Bregman divergence between positive definite matrices induced by the function $\Theta \mapsto -\log \det(\Theta)$ (Slawski & Hein, 2015). 894

A.4 PROOF FOR THEOREM 3.2

In the SAGMAN framework, we aim to construct low-dimensional manifolds for both the input and output of a GNN. For the input manifold, we use the embedding matrix $X = U_k \in \mathbb{R}^{|V| \times k}$ (as defined in Definition 3.1), where |V| is the number of nodes in the graph and k is the dimensionality of the embedding space. The goal is to learn a precision matrix Θ that captures the underlying graph structure reflected in the embeddings.

Maximum Likelihood Estimation (MLE) of the PGM (Precision Matrix). We start by formulating the MLE of the precision matrix Θ as a convex optimization problem (Dong et al., 2019):

$$\max_{\Theta} \quad F(\Theta) = \log \det(\Theta) - \frac{1}{k} \operatorname{Tr}(X^{\top} \Theta X), \tag{12}$$

where:

867

870 871

883 884 885

895 896

897

903

904

905 906 907

908 909 910

911

913

914

916

917

- 912 $\Theta = \mathcal{L} + \frac{1}{\sigma^2} I$,
 - \mathcal{L} is the graph Laplacian matrix,

ľ

- *I* is the identity matrix,
 - $\sigma^2 > 0$ is a prior variance term,
 - $Tr(\cdot)$ denotes the trace of a matrix.

Expanding the Laplacian Matrix. The graph Laplacian matrix \mathcal{L} can be decomposed as:

$$\mathcal{L} = \sum_{(p,q)\in E} w_{p,q} e_{p,q} e_{p,q}^{\top}, \tag{13}$$

where:

• E is the set of edges in the graph,

• $w_{p,q}$ is the weight of edge (p,q),

• $e_{p,q} = e_p - e_q$, with e_p being the standard basis vector corresponding to node p.

The edge weights are defined as:

$$w_{p,q} = \frac{1}{\|X^{\top} e_{p,q}\|_2^2} = \frac{1}{\|X_p - X_q\|_2^2},$$
(14)

935 when

where X_p and X_q are the embeddings of nodes p and q, respectively.

Expressing the Objective Function. Substituting Θ and \mathcal{L} into the objective function, we can split $F(\Theta)$ into two parts:

$$F = F_1 - \frac{1}{k}F_2,$$
 (15)

where:

1. First Term (F_1) :

$$F_1 = \log \det(\Theta) = \sum_{i=1}^{|V|} \log \left(\lambda_i + \frac{1}{\sigma^2}\right), \tag{16}$$

with λ_i being the *i*-th eigenvalue of the Laplacian \mathcal{L} .

2. Second Term (F_2) :

 $F_2 = \text{Tr}(X^{\top} \Theta X) = \frac{\text{Tr}(X^{\top} X)}{\sigma^2} + \sum_{(p,q) \in E} w_{p,q} \|X^{\top} e_{p,q}\|_2^2.$ (17)

The term $\frac{\text{Tr}(X^{\top}X)}{\sigma^2}$ is constant with respect to $w_{p,q}$ and can be ignored for optimization over $w_{p,q}$.

Computing Partial Derivatives. To optimize F with respect to the edge weights $w_{p,q}$, we compute the partial derivatives of F_1 and F_2 :

Derivative of F_1 with respect to edge weight:

$$\frac{\partial F_1}{\partial w_{p,q}} = \sum_{i=1}^{|V|} \frac{1}{\lambda_i + \frac{1}{\sigma^2}} \frac{\partial \lambda_i}{\partial w_{p,q}}.$$
(18)

Since $\frac{\partial \lambda_i}{\partial w_{p,q}} = v_i^\top \frac{\partial \mathcal{L}}{\partial w_{p,q}} v_i$, where v_i is the eigenvector corresponding to λ_i , and $\frac{\partial \mathcal{L}}{\partial w_{p,q}} = e_{p,q} e_{p,q}^\top$, we have:

970
971
$$\frac{\partial F_1}{\partial w_{p,q}} = \sum_{i=1}^{|V|} \frac{(v_i^\top e_{p,q})^2}{\lambda_i + \frac{1}{\sigma^2}}.$$
(19)

972 When σ approaches infinity, this expression is known as the **effective resistance distance** between 973 nodes p and q:

$$d^{\text{eff}}(p,q) = e_{p,q}^{\top} \Theta^{-1} e_{p,q}.$$
(20)

So,

$$\frac{\partial F_1}{\partial w_{p,q}} = d^{\text{eff}}(p,q). \tag{21}$$

Derivative of *F*² with respect to edge weight:

$$\frac{\partial F_2}{\partial w_{p,q}} = \|X^\top e_{p,q}\|_2^2 = \|X_p - X_q\|_2^2.$$
(22)

987 This is the **data distance** between nodes p and q:

$$d^{\text{dat}}(p,q) = \|X_p - X_q\|_2^2 = \frac{1}{w_{p,q}}.$$
(23)

Since $w_{p,q} = \frac{1}{d^{\text{dat}}(p,q)}$, we have:

$$\frac{\partial F_2}{\partial w_{p,q}} = \frac{1}{w_{p,q}}.$$
(24)

Optimization Strategy. The gradient of F with respect to $w_{p,q}$ is:

 $\frac{\partial F}{\partial w_{p,q}} = \frac{\partial F_1}{\partial w_{p,q}} - \frac{1}{k} \frac{\partial F_2}{\partial w_{p,q}} = d^{\text{eff}}(p,q) - \frac{1}{k} \frac{1}{w_{p,q}}.$ (25)

1003 To maximize F, we can:

Increase w_{p,q} when d^{eff}(p,q) > ¹/_k ¹/<sub>w_{p,q}.
Decrease w_{p,q} when d^{eff}(p,q) < ¹/_k ¹/<sub>w_{p,q}.
</sub></sub>

 However, since $w_{p,q} \ge 0$, decreasing $w_{p,q}$ effectively means pruning the edge (p,q).

Edge Pruning Strategy. We aim to prune edges where:

- Effective Resistance Distance is Small ($d^{\text{eff}}(p,q)$ is small): The nodes are well-connected in terms of the graph structure.
- Data Distance is Large $(d^{dat}(p,q)$ is large): The embeddings of the nodes are far apart.

This leads us to consider the **distance ratio** $\rho_{p,q}$:

$$\rho_{p,q} = \frac{d^{\text{eff}}(p,q)}{d^{\text{dat}}(p,q)} = w_{p,q} d^{\text{eff}}(p,q).$$
(26)

1024 Edges with small $\rho_{p,q}$ are candidates for pruning because they contribute less to maximizing *F*. By 1025 pruning such edges, we focus on retaining edges that have a significant impact on the graph's spectral properties. 1026 1027 Connection to Spectral Graph Sparsification. The ratio $\rho_{p,q}$ corresponds to the edge sampling 1028 probability used in spectral graph sparsification (Spielman & Teng, 2011). Spectral sparsification 1029 aims to approximate the original graph with a sparser graph that preserves its spectral (Laplacian) 1029 properties.

- 1030 In spectral sparsification:
 - Edges are sampled with probability proportional to $w_{p,q}d^{\text{eff}}(p,q)$.
 - Edges with higher $\rho_{p,q}$ are more likely to be included in the sparsified graph.

Therefore, our edge pruning strategy—performing spectral sparsification on the initial graph—is
 equivalent to maximize the objective function in Equation 2. This ensures that the essential structural
 properties of the graph are maintained while reducing complexity.

1039 A.5 EXPERIMENTAL SETUP 1040

See Appendix A.10 for detailed descriptions of all graph datasets used in this work. We employ the 1041 most popular backbone GNN models including GCN (Kipf & Welling, 2016), GPRGNN (Chien 1042 et al., 2020), GAT (Veličković et al., 2017), APPNP (Gasteiger et al., 2018), ChebNet (Defferrard 1043 et al., 2016), and Polynormer (Deng et al., 2024). The recommendation system is based on Pin-1044 Sage (Ying et al., 2018). Perturbations include Gaussian noise evasion attacks and adversarial attacks 1045 (DICE (Waniek et al., 2018), Nettack (Zügner et al., 2018), and FGA (Chen et al., 2018)). The input 1046 graph-based manifolds are constructed using graph adjacency and node features, while the output 1047 graph-based manifold is created using post-softmax vectors. To showcase SAGMAN's effectiveness 1048 in differentiating stable from unstable nodes, we apply SAGMAN to select 1% of the entire dataset as 1049 stable nodes, and another 1% as unstable nodes. This decision stems from that only a portion of the 1050 dataset significantly impacts model stability (Cheng et al., 2021; Hua et al., 2021; Chang et al., 2017). 1051 Additional evaluation results on the entire dataset can be found in Appendix A.12. We quantify output perturbations using cosine similarity and Kullback-Leibler divergence (KLD). Additional insights 1052 on cosine similarity, KLD, and accuracy can be found in Appendix A.7. For a large-scale dataset 1053 "ogbn-arxiv", due to its higher output dimensionality, we focus exclusively on accuracy comparisons. 1054 This decision is informed by the KLD estimator's $n^{-\frac{1}{d}}$ convergence rate (Roldán & Parrondo, 2012), 1055 where n is the number of samples and d is the dimension. In this paper, our spectral embedding 1056 method consistently utilizes the smallest 50 eigenpairs for all experiments, unless explicitly stated 1057 otherwise. 1058

1059 1060

1061 1062

1064

1032

1033

1034

1038

A.6 MEASURE DMD WITHOUT PGMS

Attack	Embedded Matrix Cosine Similarity (Stable / Unstable)
DICE level 1	0.89 / 0.89
Gaussian noise 1.0	0.96 / 0.96

Table 7: The stable (unstable) nodes identified based on traditional graph-based manifolds (Belkin & Niyogi, 2003)

1069 1070

As shown in Table 7, we cannot obtain meaningful DMDs with traditional graph-based manifolds
 (kNN graphs) adopted in the Laplacian Eigenmaps framework (Belkin & Niyogi, 2003).

1073 1074 1075

A.7 METRICS FOR ASSESSING GNN STABILITY

1076 In the context of single-label classification in graph nodes, consider an output vector $\mathbf{y} = [y_1, y_2, ..., y_k]$ corresponding to an input \mathbf{x} , where k represents the total number of classes. The model's predicted class is denoted as $\hat{y} = \operatorname{argmax}_i(y_i)$. Now, let's assume that the output vector transforms to $\mathbf{y}' = [y'_1, y'_2, ..., y'_k]$, while preserving the ordinality of the elements, i.e., if $y_i > y_j$, then $y'_i > y'_j$. This condition ensures that $\hat{y}' = \operatorname{argmax}_i(y'_i) = \hat{y}$.

Relying solely on model accuracy can be deceptive, as it is contingent upon the preservation of the ordinality of the output vector elements, even when the vector itself undergoes significant transformations. This implies that the model's accuracy remains ostensibly unaffected as long as the ranking of the elements within the output vector is conserved. However, this perspective neglects potential alterations in the model's prediction confidence levels.

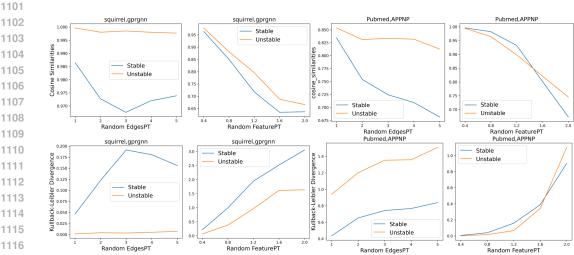
In contrast, the cosine similarity provides a more holistic measure as it quantifies the angle between two vectors, thereby indicating the extent of modification in the output direction. This method offers a more granular insight into the impact of adversarial attacks on the model's predictions.

Moreover, it is crucial to consider the nature of the output space, Y. In situations where Y forms a probability distribution, a common occurrence in classification problems, the application of a distribution distance measure such as the Kullback-Leibler (KL) divergence is typically more suitable. Unlike the oversimplified perspective of accuracy, these measures can provide a nuanced understanding of the degree of perturbation introduced in the predicted probability distribution by an adversarial attack. This additional granularity can expose subtle modifications in the model's output that might be missed when solely relying on accuracy as a performance metric.

1095

A.8 GNN STABILITY ANALYSIS WITHOUT GDR

In this study, we present the outcomes of stability quantification using original input and output graphs, as depicted in Figure 5. Our experimental findings underscore a key observation: SAGMAN without GDR does not allow for meaningful estimations of the GNN stability.



1117 1118

1119 Figure 5: The horizontal axes, denoted by X, represent the magnitude of perturbation applied. 'Random EdgesPT' refers to the DICE adversarial attack scenario, in which pairs of nodes with 1120 different labels are connected and pairs with the same label are disconnected, with the number of 1121 pairs being equal to X. 'Random FeaturePT' indicates the application of Gaussian noise perturbation, 1122 expressed as $FM + X\eta$, where FM denotes the feature matrix and η represents Gaussian noise. 1123 The upper and lower subfigures illustrate the cosine similarity and the Kullback-Leibler Divergence 1124 (KLD). 'Stable/Unstable' denotes the samples that are classified as stable or unstable without GDR, 1125 respectively. 1126

1120

1129

1128 <u>д</u> с

A.9 FAST EFFECTIVE-RESISTANCE ESTIMATION FOR LRD-BASED GRAPH DECOMPOSITION

1130 The effective-resistance between nodes $(p,q) \in |V|$ can be computed using the following equation: 1131

$$d^{eff}(p,q) = \sum_{i=2}^{N} \frac{(u_i^{\top} e_{p,q})^2}{u_i^{\top} L_G u_i},$$
(27)

1140

1141 1142

1148

1149

1156 1157

1158 1159

1165

1166

1176

1179

1182

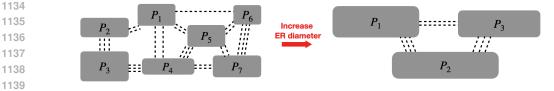


Figure 6: Graph decomposition results with respect to effective-resistance (ER) diameter

1143 where u_i represents the eigenvector corresponding to σ_i eigenvalue of L_G and $e_{p,q} = e_p - e_q$. To 1144 avoid the computational complexity associated with computing eigenvalues/eigenvectors, we leverage 1145 a scalable algorithm that approximates the eigenvectors by exploiting the Krylov subspace. In this 1146 context, given a nonsingular matrix $A_{N \times N}$ and a vector $c \neq 0 \in \mathbb{R}^N$, the order-(m) Krylov subspace 1147 generated by A from c is defined as:

$$\kappa_m(A,c) := span(c, Ac, A^2c, ..., A^{m-1}c),$$
(28)

where c denotes a random vector, and A denotes the adjacency matrix of graph G. We compute a new set of vectors denoted as $x^{(1)}, x^{(2)}, ..., x^{(m)}$ by ensuring that the Krylov subspace vectors are mutually orthogonal with unit length. We estimate the effective-resistance between node p and q using Equation 27 by exploring the eigenspace of L_G and selecting the vectors that capture various spectral properties of G:

$$d^{eff}(p,q) \approx \sum_{i=1}^{m} \frac{(x^{(i)^{\top}} e_{p,q})^2}{x^{(i)^{\top}} L_G x^{(i)}},$$
(29)

1160 We control the diameter of each cycle by propagating effective resistances across multiple levels. 1161 Let G = (V, E) represent the graph at the δ -th level, and let the edge $(p, q) \in E$ be a contracted 1162 edge that creates a supernode $\vartheta \in V^{(\delta+1)}$ at level $\delta + 1$. We denote the vector of node weights as 1163 $\eta^{(\delta)} \in \mathbb{R}_{\geq 0}^{V^{(\delta)}}$, which is initially set to all zeros for the original graph. The update of η at level $\delta + 1$ is 1164 defined as follows:

$$\eta_{\vartheta} := \eta(p^{(\delta)}) + \eta(q^{(\delta)}) + d_{eff}^{(\delta)}(p,q).$$
(30)

1167 Consequently, the effective-resistance diameter of each cycle is influenced not only by the computed 1168 effective-resistance $(d_{eff}^{(\delta)})$ at the current level but also by the clustering information acquired from 1169 previous levels.

The graph decomposition results with respect to effective-resistance (ER) diameter are illustrated in Figure 6. The figure demonstrates that selecting a larger ER diameter leads to the decomposition of the graph into a smaller number of partitions, with more nodes included in each cluster. On the left side of the figure, the graph is decomposed into seven partitions: $P_1, ..., P_7$, by choosing a smaller ER diameter. Conversely, increasing the ER diameter on the right side of the figure results in the graph being partitioned into three clusters: P_1, P_2 , and P_3 .

A.10 ADDITIONAL RESULTS FOR GNN STABILITY EVALUATION AND STATISTICS OF DATASETS

We present the additional results in Figure 8, Figure 9, Figure 10, Figure 7, Table 8, and Table 9.Table 10 summarizes the datasets utilized.

1183	Table 8: Robustness Evaluation	of GAT u	nder PGD	Attack on Co	ora
1184	PGD Perturbation	0.05	0.10	0.15	
1185 1186	Robust Accuracy	1.0000	1.0000	1.0000	
1187	Non-Robust Accuracy	0.9630	0.8889	0.8148	

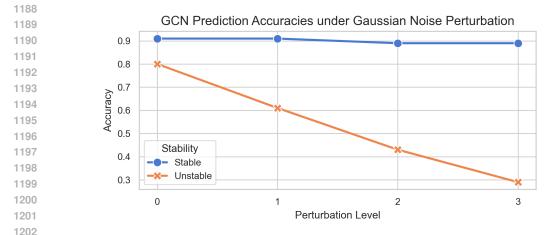


Figure 7: SAGMAN-selected stable/unstable samples for the "ogbn-arxiv" dataset. We report the GCN prediction accuracies under different levels of Gaussian Noise Perturbation $FM + X\eta$, where FM denotes the feature matrix, η represents Gaussian noise, and X is the noise perturbation level.

Table 9: Nettack adversarial attack targeting selected Cora samples in GCN

Nettack Level	Cosine Similarities: Stable/Unstable
1	0.99/0.90
2	0.98/0.84
3	0.97/0.81

1216 A.11 WHY GENERALIZED EIGENPAIRS ASSOCIATE WITH DMD

(Cheng et al., 2021) propose a method to estimate the maximum distance mapping distortion (DMD), denoted as δ_{max}^{M} , by solving the following combinatorial optimization problem:

$$\max \delta^{M} = \max_{\substack{\forall p,q \in V \\ p \neq q}} \frac{e_{p,q}^{\top} L_{Y}^{+} e_{p,q}}{e_{p,q}^{\top} L_{X}^{+} e_{p,q}}$$
(31)

When computing δ_{max}^{M} via effective-resistance distance, the stability score is an upper bound of δ_{max}^{M} (Cheng et al., 2021).

1227 A function Y = M(X) is called Lipschitz continuous if there exists a real constant $K \ge 0$ such that 1228 for all $x_i, x_j \in X$:

1229 1230 1231

1235 1236

1207

1217

1220

1222 1223 1224

$$dist_Y(M(x_i), M(x_j)) \le K dist_X(x_i, x_j), \tag{32}$$

where K is the Lipschitz constant for the function M. The smallest Lipschitz constant, denoted by K^* , is called the best Lipschitz constant. Let the resistance distance be the distance metric, then (Cheng et al., 2021):

$$\Lambda_{max}(L_Y^+ L_X) \ge K^* \ge \delta_{max}^M. \tag{33}$$

1237 Equation 33 indicates that the $\lambda_{max}(L_Y^+L_X)$ is also an upper bound of the best Lipschitz constant 1238 K^* under the low dimensional manifold setting. A greater $\lambda_{max}(L_Y^+L_X)$ of a function (model) 1239 implies worse stability since the output will be more sensitive to small input perturbations. A node 1240 pair (p,q) is deemed non-robust if it exhibits a large DMD, i.e., $\delta^M(p,q) \approx \delta_{max}^M$. This suggests 1241 that a non-robust node pair consists of nodes that are adjacent in the G_X but distant in the G_Y . 126 To effectively identify such non-robust node pairs, the Cut Mapping Distortion (CMD) metric was

1242 1243

Table 10: Summary of datasets used in our experiments

1 10	iuoi	fuele for Summing of autoete acea in our enperimente						
1244	Dataset	Туре	Nodes	Edges	Classes	Features		
1245	Cora	Homophily	2,485	5,069	7	1.433		
1246	Cora-ML	Homophily	2,810	7.981	7	2,879		
1247	Pubmed	Homophily	19,717	44.324	3	500		
1248	Citeseer	Homophily	2,110	3,668	6	3,703		
1249	Chameleon	Heterophily	2,277	62,792	5	2,325		
1250	Squirrel	Heterophily	5,201	396,846	5	2,089		
1251	ogbn-arxiv	Homophily	169,343	1,166,243	40	128		
1252								

1253

1257

1259

1254 introduced. For two graphs G_X and G_Y sharing the same node set V, let $S \subset V$ denote a node subset and \overline{S} denote its complement. Also, let $cut_G(S,\overline{S})$ denote the number of edges crossing S 1255 and S in graph G. The CMD $\zeta(S)$ of node subset S is defined as (Cheng et al., 2021): 1256

$$\zeta(S) \stackrel{\text{def}}{=} \frac{cut_{G_Y}(S,\bar{S})}{cut_{G_X}(S,\bar{S})}.$$
(34)

A small CMD score indicates that node pairs crossing the boundary of S are likely to have small distances in G_X but large distances in G_Y . 1261

1262 Given the Laplacian matrices L_X and L_Y of input and output graphs, respectively, the minimum 1263 CMD ζ_{\min} satisfies the following inequality:

$$\zeta_{\min} = \min_{\forall S \subset V} \zeta(S) \ge \frac{1}{\sigma_{\max}(L_Y^+ L_X)}$$
(35)

1265 1266 1267

1273

1282

1283

1286 1287 1288

1294

1295

1264

Equation 35 establishes a connection between the maximum generalized eigenvalue $\sigma_{\max}(L_Y^+L_X)$ 1268 and ζ_{\min} , indicating the ability to exploit the largest generalized eigenvalues and their corresponding 1269 eigenvectors to measure the stability of node pairs. Embedding G_X with generalized eigenpairs. We 1270 first compute the weighted eigensubspace matrix $V_s \in \mathbb{R}^{N \times s}$ for spectral embedding on G_X with N 1271 nodes: 1272

$$V_s \stackrel{\text{def}}{=} \left[v_1 \sqrt{\sigma_1}, \dots, v_s \sqrt{\sigma_s} \right],\tag{36}$$

where $\sigma_1, \sigma_2, ..., \sigma_s$ represent the first s largest eigenvalues of $L_Y^+ L_X$ and $v_1, v_2, ..., v_s$ are the 1274 corresponding eigenvectors. Consequently, the input graph G_X can be embedded using V_s , so each node is associated with an s-dimensional embedding vector. We can then quantify the stability of 1276 an edge $(p,q) \in E_X$ by measuring the spectral embedding distance of its two end nodes p and q. 1277 Formally, we have the edge stability score defined for any edge $(p,q) \in E_X$ as $stability^M(p,q) \stackrel{\text{def}}{=}$ 1278 $||V_s^{\top}e_{p,q}||_2^2$ Let $u_1, u_2, ..., u_s$ denote the first s dominant generalized eigenvectors of $L_X L_Y^+$. If an 1279 edge (p,q) is dominantly aligned with one dominant eigenvector u_k , where $1 \le k \le r$, the following 1280 holds: 1281

 $(u_i^{\top} e_{p,q})^2 \approx \begin{cases} \alpha_k^2 \gg 0 & \text{ if } (i=k) \\ 0 & \text{ if } (i \neq k). \end{cases}$ (37)

Then its edge stability score has the following connection with its DMD computed using effective-1284 resistance distances (Cheng et al., 2021): 1285

$$\|V_s^{\top} e_{p,q}\|_2^2 \propto \left(\delta^M(p,q)\right)^3.$$
(38)

The stability score of an edge $(p,q) \in E_X$ can be regarded as a surrogate for the directional derivative 1289 $\|\nabla_v M(x)\|$ under the manifold setting, where $v = \pm (x_p - x_q)$. An edge with a larger stability score 1290 is considered more non-robust and can be more vulnerable to attacks along the directions formed by 1291 its end nodes.

Last, the node stability score can be calculated for any node (data sample) $p \in V$ as follows: 1293

 $score(p) = \frac{1}{|\mathbb{N}_X(p)|} \sum_{q_i \in \mathbb{N}_X(p)} \left(\|V_s^\top e_{p,q}\|_2^2 \right) \propto \frac{1}{|\mathbb{N}_X(p)|} \sum_{q_i \in \mathbb{N}_Y(p)} \left(\delta^M(p,q_i) \right)^3$ (39) where $q_i \in \mathbb{N}_X(p)$ denotes the *i*-th neighbor of node *p* in graph G_X , and $\mathbb{N}_X(p) \in V$ denotes the node set including all the neighbors of *p*. The DMD score of a node (data sample) *p* can be regarded as a surrogate for the function gradient $\|\nabla_x M(p)\|$ where *x* is near *p* under the manifold setting. A node with a larger stability score implies it is likely more vulnerable to adversarial attacks.

1300 1301

1302

1311

A.12 VARIOUS SAMPLING SCHEMES FOR SAGMAN-GUIDED PERTURBATIONS

Previous works (Cheng et al., 2021; Hua et al., 2021; Chang et al., 2017) highlighted that only 1303 part of the dataset plays a crucial role in model stability, so we want to focus on the difference 1304 between the most "stable" and "unstable" parts. However, it is certainly feasible to evaluate the entire 1305 graph. Table 11 shows the result regarding the Pubmed dataset in GPRGNN under Gaussian noise 1306 perturbation. Samples were segmented based on SAGMAN ranking, with the bottom 20% being the 1307 most "stable", the middle 60% as intermediate, and the top 20% representing the most "unstable". As 1308 anticipated, the "stable" category (representing the bottom 20%) should exhibit the lowest average 1309 KL divergences. This is followed by the intermediate category (covering the mid 60%), and finally, 1310 the "unstable" category (comprising the top 20%) should display the highest divergences.

Table 11: KLD across varying Gaussian noise perturbations, expressed as $FM + X\eta$, where FMdenotes the feature matrix, η represents Gaussian noise, and X denotes the perturbation level. The dataset is divided into three segments based on the stability ranking of nodes as determined by SAGMAN.

Perturbation Level	KL divergence (bottom 20%)	KL divergence (mid 60%)	KL divergence (top 20%)
0.4	0.01	0.03	0.03
0.8	0.09	0.16	0.19
1.2	0.43	0.56	0.59

1323 A.13 SAGMAN'S RUNTIME ACROSS DATASETS 1324

Figure 11 demonstrates the high efficiency of SAGMAN in processing large graphs, attributing its performance to the near-linear time complexity of its components.

- 1327
- 1328

1330

A.14 HYPERPARAMETER STUDY OF SAGMAN

1331 In this section, we present a hyperparameter study of the SAGMAN framework to evaluate the impact 1332 of key parameters on its performance. Specifically, we analyze how varying the number of nearest 1333 neighbors k used to construct the initial graph and the sparsification parameter *sparse_numer* affect 1334 the stability assessment and robustness of GNNs.

1335 1336

1337

1345

A.14.1 IMPACT OF k AND sparse_numer

1338 The hyperparameter k determines the number of nearest neighbors in the k-nearest neighbor (KNN) 1339 algorithm used to construct the initial graph for the manifold. The parameter *sparse_numer* controls 1340 the level of sparsification during graph pruning, influencing the density and connectivity of the 1341 resulting graph.

To assess the effects of these hyperparameters, we conducted experiments on the Cora dataset using a GCN model. We varied k and *sparse_numer* while measuring the following metrics:

- **PGD Attack Accuracy (Stable Nodes)**: The classification accuracy on stable nodes after applying a PGD attack.
- PGD Attack Accuracy (Unstable Nodes): The classification accuracy on unstable nodes after applying a PGD attack.
- **Cosine Similarity (Stable Nodes)**: The average cosine similarity between the original and perturbed embeddings of stable nodes.

• **Cosine Similarity (Unstable Nodes)**: The average cosine similarity between the original and perturbed embeddings of unstable nodes.

1355 A.14.2 RESULTS AND DISCUSSION

Table 12 summarizes the results of our experiments. We varied k from 10 to 80 and *sparse_numer* from 2 to 5.

Table 12: Impact of k and *sparse_numer* on SAGMAN's performance. 'NC' denotes configurations where ARPACK did not converge.

2	k sparse_numer		PGD Acc. (Stable)	PGD Acc. (Unstable)	Cosine Sim. Diff.	
3	10	2	1.00	0.74	0.99998 / 0.98302	
4	10	3	1.00	0.96	0.99985 / 0.99983	
5	10	4	0.89	1.00	0.99985 / 0.99987	
6	30	2	1.00	0.74	0.99996 / 0.98636	
7	30	3	1.00	0.81	0.99998 / 0.98579	
8	30	4	1.00	0.74	0.99993 / 0.98528	
0	50	3	1.00	0.81	0.99964 / 0.99986	
9	50	4	0.93	0.81	0.99313 / 0.99965	
0	50	5	1.00	0.89	0.99980 / 0.99979	
1	80	2	0.96	0.89	0.99998 / 0.99722	
2	80	3	0.96	0.81	0.99999 / 0.99809	
3	80	4	1.00	0.74	0.99968 / 0.99678	

¹³⁷³ 1374 1375

1350

1351

1352 1353 1354

1367

Effect of k: - When k is small (e.g., k = 10), the initial graph captures local relationships but may miss some global structural information. - As k increases to 30 and 50, the performance on stable nodes remains high, and the cosine similarity between original and perturbed embeddings for stable nodes remains close to 1.0, indicating robustness. - A larger k (e.g., k = 80) does not necessarily lead to better performance and may cause computational challenges, as indicated by non-converging configurations (not shown in the table).

Effect of sparse_numer: - Lower values of sparse_numer (e.g., 2 or 3) result in sparser graphs after pruning, which helps in maintaining high classification accuracy and robustness on stable nodes. - Increasing sparse_numer to 4 or 5 leads to denser graphs, which may capture more complex structures but can also introduce noise, potentially affecting stability. - Configurations with sparse_numer = 5 sometimes led to convergence issues during eigenvalue computations, suggesting that overly dense graphs may pose computational difficulties.

Cosine Similarity Analysis: - The cosine similarity between the original and perturbed embeddings is consistently higher for stable nodes compared to unstable nodes. - For example, with k = 10 and *sparse_numer* = 2, the cosine similarity is 0.99998 for stable nodes and 0.98302 for unstable nodes, highlighting SAGMAN's ability to distinguish between stable and unstable nodes.

1393

1388

1394

A.15 ROBUSTNESS UNDER POISONING ATTACKS AND COMPARISON WITH LIPSCHITZ-BASED METHODS

In this section, we compare the robustness of SAGMAN with a Lipschitz-based stability method, specifically the LipReLU method (Jia et al., 2023), under poisoning attacks. While previous work (Jia et al., 2023) focuses exclusively on poisoning attacks, SAGMAN is primarily designed for evasion attacks. However, due to its versatility, SAGMAN can be deployed in poisoning scenarios and combined with other robustness techniques.

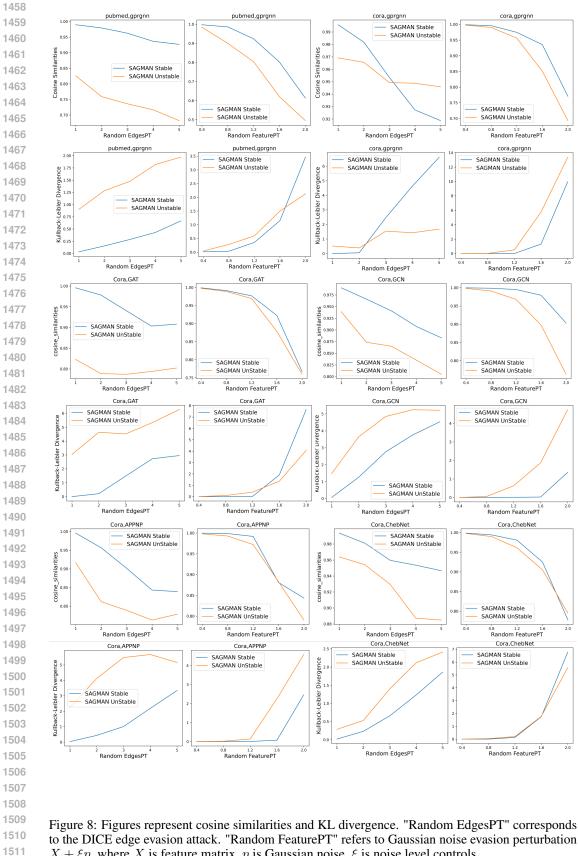
¹⁴⁰³ To demonstrate this, we conducted experiments using the DICE poisoning attack on the Cora dataset with a GCN model. We evaluated the robustness improvement provided by SAGMAN, LipReLU,

and a combination of both methods. The results highlight the accuracy improvement on the 10% most unstable samples, as identified by SAGMAN.

1408Table 13: Accuracy comparison under DICE poisoning attack for different numbers of edge perturba-
tions. Best results are highlighted in **bold**.

1410	Method	1 Edge	10 Edges	50 Edges	100 Edges	
1411	LipReLU	0.7862	0.7903	0.7782	0.7822	
1412	SÂGMAN	0.8588	0.8427	0.8508	0.8548	
1413	LipReLU + SAGMAN	0.8468	0.8467	0.8467	0.8427	
1414						

The results in Table 13 demonstrate that SAGMAN outperforms the Lipschitz-based method LipReLU in most cases, particularly as the number of edge perturbations increases. Combining SAGMAN with LipReLU also yields competitive results, indicating that SAGMAN can enhance the robustness provided by Lipschitz-based methods. This suggests that SAGMAN is a versatile plug-in that can be effectively integrated with existing robustness techniques to improve GNN resilience under poisoning attacks.



 $X + \xi \eta$, where X is feature matrix, η is Gaussian noise, ξ is noise level controls

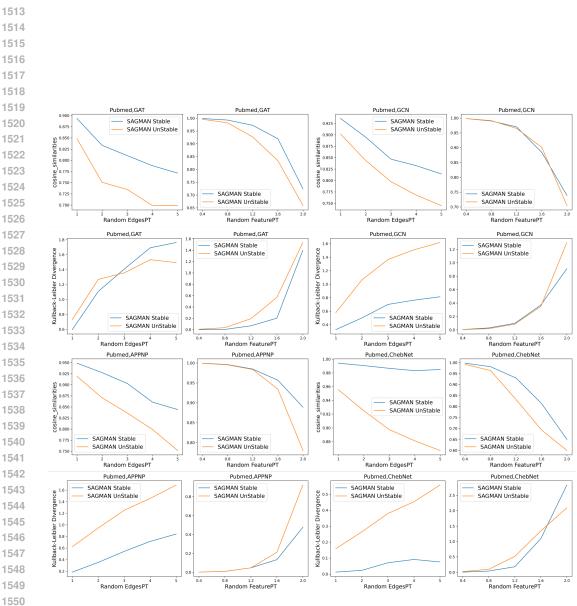


Figure 9: The horizontal axes, denoted by X, represent the magnitude of perturbation applied. 'Random EdgesPT' refers to the DICE adversarial attack scenario, in which pairs of nodes with different labels are connected and pairs with the same label are disconnected, with the number of pairs being equal to X. 'Random FeaturePT' indicates the application of Gaussian noise perturbation, expressed as $FM + X\eta$, where FM denotes the feature matrix and η represents Gaussian noise. The upper and lower subfigures illustrate the cosine similarity and the Kullback-Leibler Divergence (KLD). 'SAGMAN Stable/Unstable' denotes the samples that are classified as stable or unstable by SAGMAN, respectively.

