Implications of sparsity and high triangle density for graph representation learning

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Talk structure

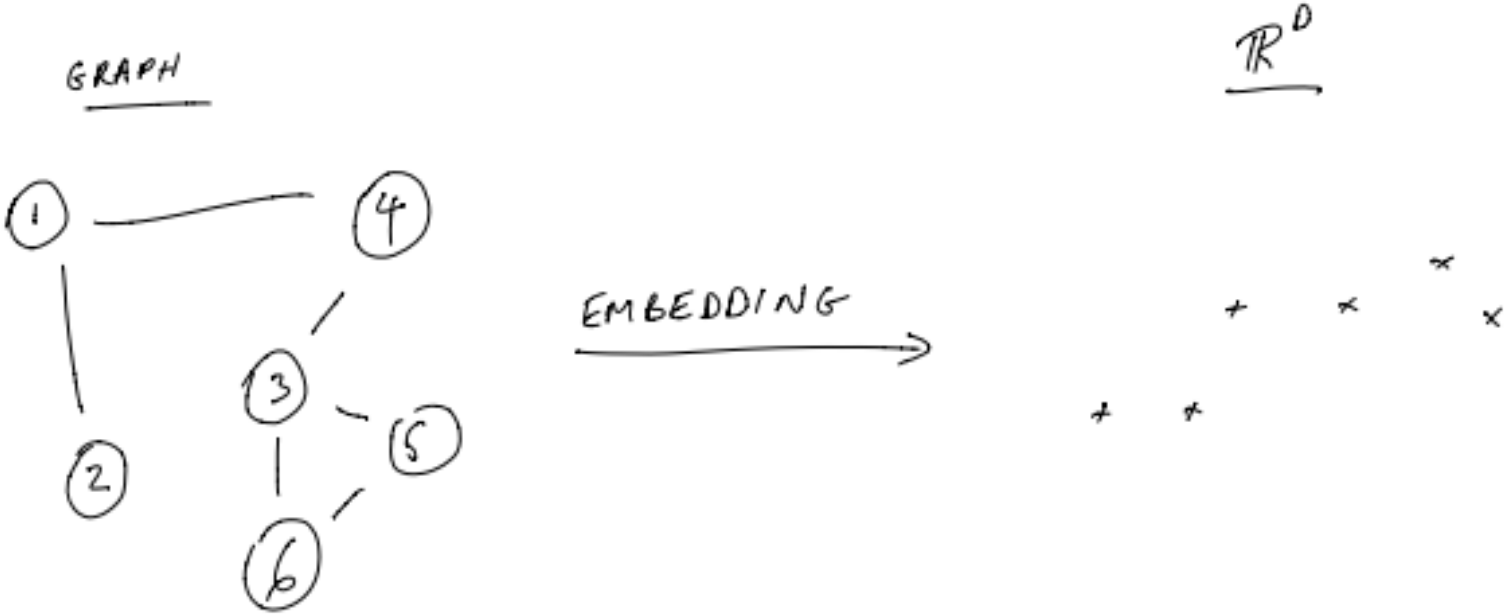
Mathematical prerequisites

Motivating work

Main result

Implications

Graph embedding



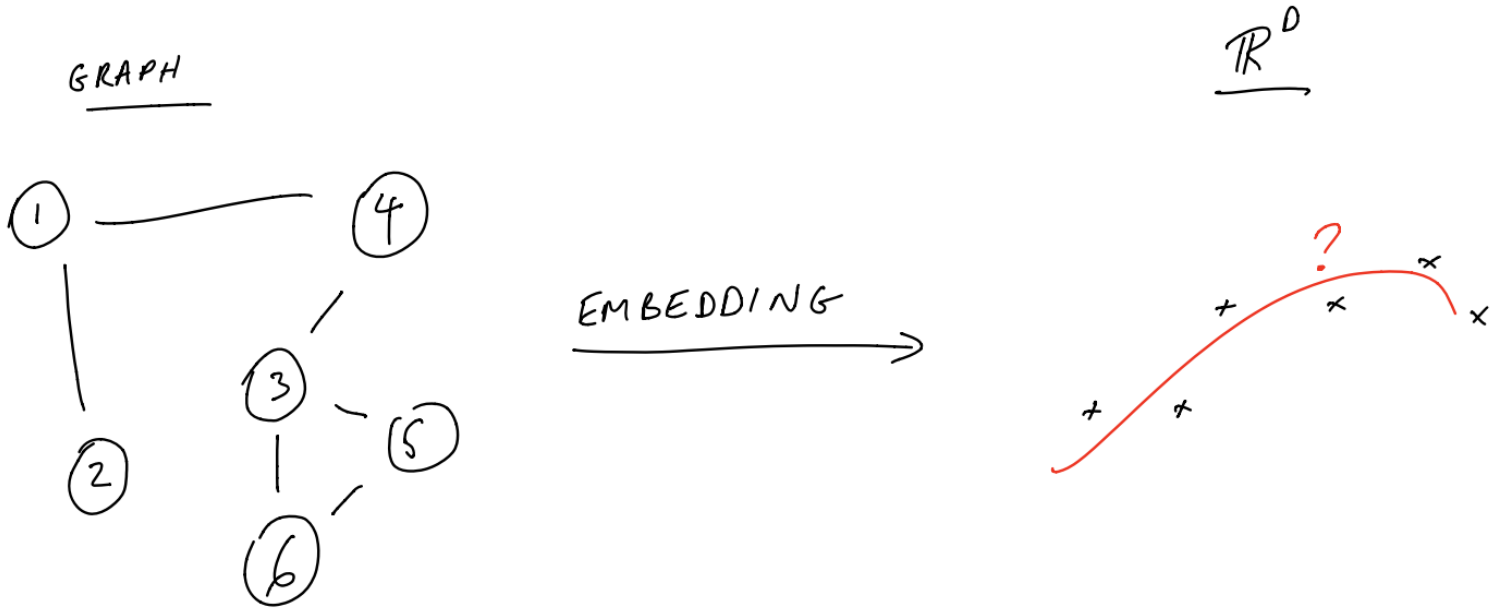
Adjacency spectral embedding

Input symmetric adjacency matrix $\mathbf{A}$ Compute $\mathbf{A} \approx \hat{\mathbf{X}}\hat{\mathbf{X}}^\top$ with

$\hat{\mathbf{X}} = [\hat{X}_1, \ldots, \hat{X}_n]^\top \in \mathbb{R}^{n \times D}$:

- compute truncated spectral decomposition $\mathbf{A} \approx \hat{\mathbf{U}}\hat{\mathbf{S}}\hat{\mathbf{V}}^\top$
- let $\hat{\mathbf{X}} = \hat{\mathbf{U}}\hat{\mathbf{S}}^{1/2}$

The manifold hypothesis



(Rubin-Delanchy, 2020)

Latent position model

Suppose the nodes have true latent positions $Z_1, \ldots, Z_n \in \mathcal{Z}_n$, where $\mathcal{Z}_n \subseteq \mathbb{R}^d$ is a compact topological manifold, and are i.i.d. from a probability distribution G_n.

Let $f : \mathcal{Z}_n \times \mathcal{Z}_n \to [0, 1]$ be a symmetric positive-definite function, called a kernel.

Next, suppose the graph's adjacency matrix satisfies

$$\mathbf{A}_{ij}^{(n)} \overset{ind}{\sim} \text{Bernoulli}\left\{f(Z_i, Z_j)\right\},$$

for $i < j$.

How is Z_i related to $\hat{X}_i$?

Random dot product graph (RDPG)

$\hat{X}_i$ estimates X_i, where

$$\mathbf{A}_{ij}^{(n)} \overset{ind}{\sim} \text{Bernoulli}\left\{\langle X_i, X_j \rangle\right\}, \quad \text{for } i < j,$$

and $\langle \cdot, \cdot \rangle$ denotes the (possibly indefinite) inner product, a model known as the (generalised) random dot product graph (Rubin-Delanchy et al., 2017).

Claim: The X_i are a high-dimensional but somehow faithful transformation of Z_i,

$$X_i = \phi(Z_i).$$

Infinite-dimensional RDPG

The inner product can be used to represent any positive definite kernel f (although typically in infinite dimension) using the associated Mercer feature map $\phi : \mathcal{Z}_n \to \mathbb{R}^{\mathbb{N}}$,

$$\langle \phi(x), \phi(y) \rangle = f(x, y), \quad \text{for all } x, y \in \mathcal{Z}_n,$$

defining $X_i := \phi(Z_i)$. Therefore, the latent position model also defines an infinite-dimensional RDPG.

Theorem

The map ϕ is a bi-Lipschitz homeomorphism. As a result, the X_i are supported on a topological manifold $\mathcal{M}_n := \phi(\mathcal{Z}_n)$ of the same dimension as $\mathcal{Z}_n$.

(Whiteley et al., 2021)

Motivating work

PNAS

RESEARCH ARTICLE | COMPUTER SCIENCES |

The impossibility of low-rank representations for triangle-rich complex networks

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Intuition

Under a random dot product graph,

$$\mathbf{A}_{ij}^{(n)} \overset{ind}{\sim} \text{Bernoulli}\left\{\langle X_i, X_j \rangle\right\},$$

- the graph is sparse if most inner products are small
- inner products are small if either the X_i are small (low norm) or they are 'almost orthogonal'
- but we can't have arbitrarily many 'almost orthogonal' vectors in $\mathbb{R}^D$
- so for low D and large n, the X_i must be small to achieve sparsity, making triangles almost impossible

Sparsity and triangle density

Under a random dot product graph with i.i.d. latent positions X_i, define the graph sparsity factor, ρ_n, and triangle density, Δ_n, via

$$n\rho_n = n \iint \langle x, y \rangle F_n(x) F_n(y), \quad \text{(expected degree)}$$

$$n\Delta_n = \binom{n}{3} \iiint \langle x, y \rangle \langle y, z \rangle \langle z, x \rangle F_n(x) F_n(y) F_n(z),$$

(expected number of triangles)

where F_n is the distribution of $X_1, \ldots, X_n$.

Question

Can a random dot product graph be sparse, i.e., $\rho_n = o(1)$, with high triangle density, i.e., $\Delta_n = \Omega(1)$?

1. The answer is *no* if X_i are finite-dimensional (Seshadhri et al.), but:
2. The answer is *yes* if X_i are infinite-dimensional, yet supported on a low-dimensional manifold.

Proof approach

- Start with a compact topological manifold $\mathcal{Z}_n$, e.g. unit cube/sphere,
- build manifold $\mathcal{M}_n$ using a homeomorphism $\mathcal{M}_n := \phi(\mathcal{Z}_n)$ which is non-distortive,
- this results in $\mathcal{M}_n$ being a manifold of the same dimension as $\mathcal{Z}_n$,
- then can push forward a probability distribution G_n on $\mathcal{Z}_n$ to $\mathcal{M}_n$ using ϕ to get an identical distribution F_n on $\mathcal{M}_n$

We do this for settings which give a random graph with calculable sparsity and triangle density.

Calculation of sparsity and triangle density

Let $f : \mathcal{Z}_n \times \mathcal{Z}_n \to [0,1]$ be a positive-definite kernel which is Lipschitz continuous in each variable, with eigenvalues λ_k with respect to G_n, and Mercer feature map ϕ.

Lemma

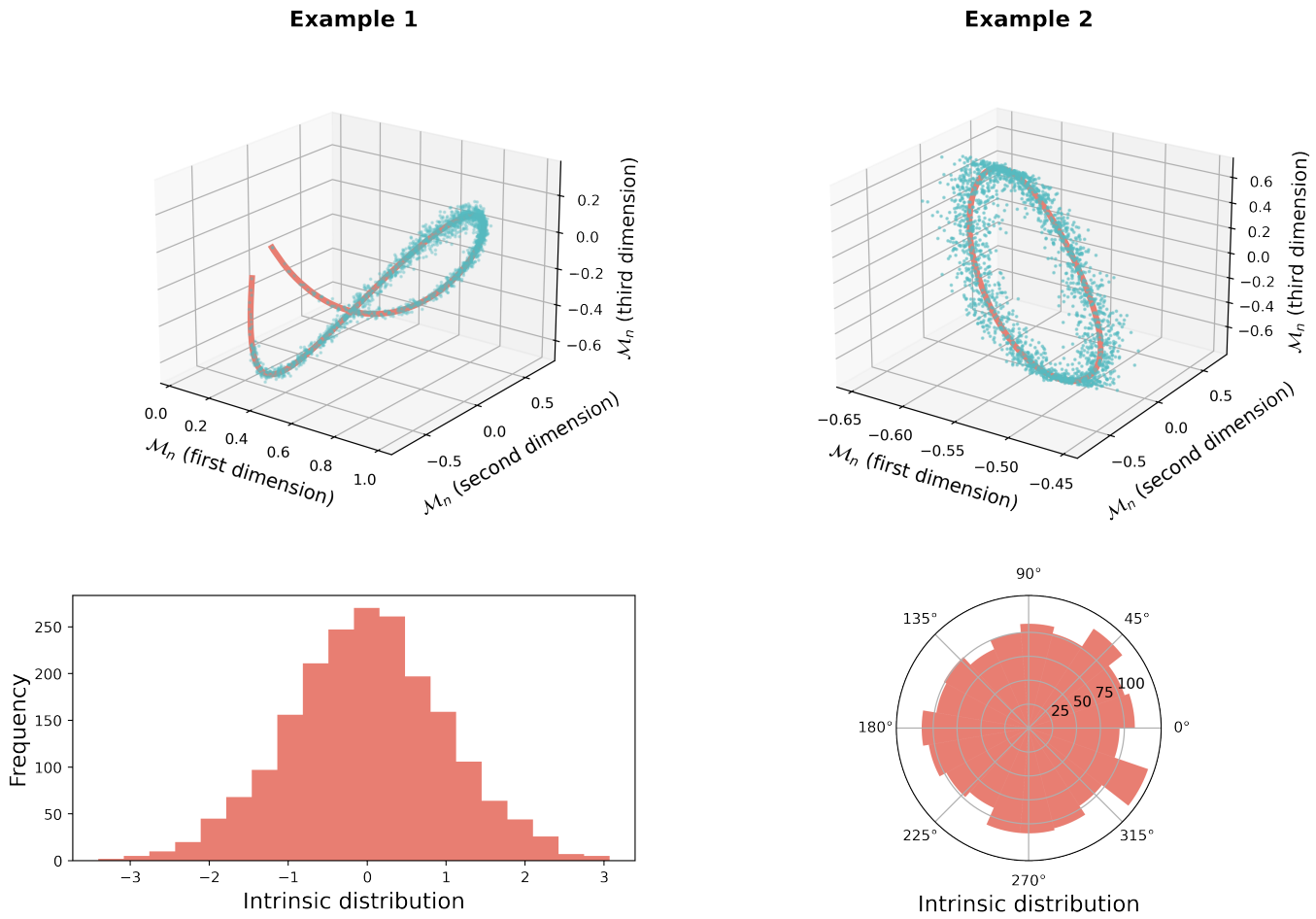
$$\iiint f(x,y)f(y,z)f(z,x)G_n(x)G_n(y)G_n(z) = \sum_{k=1}^{\infty} \lambda_k^3.$$

For the random dot product graph with $F_n = \phi(G_n)$,

$$\rho_n = \iint f(x,y)G_n(x)G_n(y), \qquad \text{and} \qquad \Delta_n = \Theta\left(n^2\right) \sum_{k=1}^{\infty} \lambda_k^3.$$

Results

In explicit examples, we can achieve $\rho_n = O(1/n)$ (constant expected degree) and $\Delta_n = \Omega(1)$ with e.g. normal or uniform on-manifold distributions



Triangles and community structure

It is known that certain forms of community structure do not result in triangles, i.e.

$$\text{community structure} \not\Longrightarrow \text{high triangle density.}$$

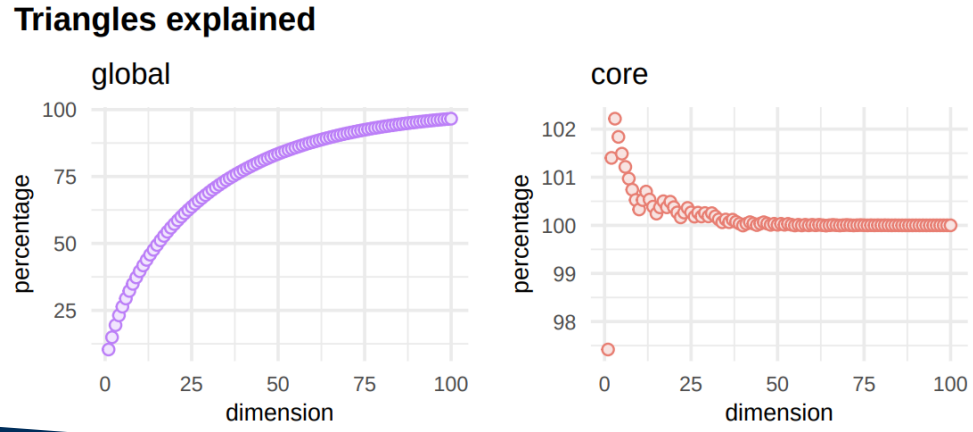
There is a perception that the reverse implication is true. Our constructions achieve high triangle density when no sensible notion of community structure is present, i.e.

$$\text{high triangle density} \not\Longrightarrow \text{community structure.}$$

Global vs local embedding

Representing a sparse graph, $n\rho_n = o(\log n)$, on a low-dimensional manifold leaves large parts of the manifold uncovered. Therefore, fully identifying the manifold is, in general, impossible.

By 'zooming in' on a small neighbourhood of the graph, we can form an embedding that represents a flat approximation of the manifold over that region.



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