Two-sample hypothesis testing for random dot product graphs

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Introduction and Overview

1. The problem of deciding whether two given graphs are the “same” has applications in e.g., neuroscience, social networks.

2. We propose a valid and consistent test for the above under a random graph model.

3. The test proceeds by embedding the graphs into Euclidean space followed by computing a distance between a kernel density “estimate” of the embedded points.
Random dot product graphs

Let $\Omega$ be a subset of $\mathbb{R}^d$ such that, for all $\omega, \omega' \in \Omega$, $0 \leq \langle \omega, \omega' \rangle \leq 1$. Let $F$ be a distribution taking values in $\Omega$.

1. Let $\{X_i\}_{i=1}^n \overset{i.i.d.}{\sim} F$.

2. $A_n \sim \text{RDPG}(F)$ is the adjacency matrix of a graph associated with $\{X_i\}_{i=1}^n$. The upper diagonal entries of $A_n$ are independent Bernoulli random variables with $\mathbb{P}[X_i \sim X_j] = \langle X_i, X_j \rangle$, i.e.,

$$
\mathbb{P}[A_n | \{X_i\}_{i=1}^n] = \prod_{i<j} \langle X_i, X_j \rangle^{A_n(i,j)} (1 - \langle X_i, X_j \rangle)^{1-A_n(i,j)}
$$

See Young and Scheinerman (2007).
Random dot product graphs are an example of latent position graphs (Hoff et al., 2002), in which each vertex is associated with a latent position.

Random dot product graphs are related to stochastic blockmodels Holland et al. (1983), degree-corrected stochastic block models Karrer and Newman (2011), and mixed membership block models Airoldi et al. (2008).

Non-identifiability: For any distribution $F$ and orthogonal matrix $W$, the graphs $A \sim \text{RDPG}(F)$ and $B \sim \text{RDPG}(F \circ W)$ are identically distributed.
\[ X = \{X_i\}_{i=1}^n \subset \mathbb{R}^d \]

original latent vectors

\[ P = XX^T \in [0, 1]^{n \times n} \]
probability matrix

\[ A = \text{Bern}(K) \]
adjacency matrix

**Observation**

A looks like P (at least at rough scale).
Problem Statement

Given $A \sim \text{RDPG}(F)$ and $B \sim \text{RDPG}(G)$, consider the following test:

$$
\mathcal{H}_0: F =_W G \quad \text{against} \quad \mathcal{H}_1: F \neq_W G
$$

where $F =_W G$ denotes that there exists an orthogonal $d \times d$ matrix $W$ such that $F = G \circ W$ and $F \neq_W G$ denotes that $F \neq G \circ W$ for any orthogonal $W$. 
Adjacency spectral embedding

Definition

Let $A$ be an $n \times n$ adjacency matrix and denote by $|A|$ the matrix $(A^T A)^{1/2}$. Let $d \geq 1$ and consider the following spectral decomposition of $|A|

|A| = [U_A \tilde{U}_A][S_A \oplus \tilde{S}_A][U_A \tilde{U}_A]

where $U_A \in \mathbb{R}^{n \times d}$, $\tilde{U}_A \in \mathbb{R}^{n \times d}$. The columns of $U_A$ correspond to the $d$ largest eigenvalues of $|A|$. The adjacency spectral embedding of $A$ into $\mathbb{R}^d$ is then the $n \times d$ matrix $\hat{X} = U_A S_A^{1/2}$. 
\( \hat{X} \) is close to \( X \)
Suppose $(A, X) \sim \text{RDPG}(F)$ is a graph on $n$ vertices. Denote by $\hat{X}$ the adjacency spectral embedding of $A$ into $\mathbb{R}^d$. Let $\eta > 0$ be arbitrary. Then for sufficiently large $n$ there exists a $d \times d$ orthogonal matrix $W$ such that, with probability at least $1 - 3\eta$,

$$
\left\| \hat{X} - XW \right\|_F - C_1(F) \leq \frac{C_2(F)d^{3/2} \log (n/\eta)}{\sqrt{n}}
$$

(1)

where $C_1(F)$ and $C_2(F)$ are constants depending only on $F$. 


Two-sample testing via maximum mean discrepancy

Let $\kappa$ be a kernel on $\Omega$ with reproducing kernel Hilbert space $\mathcal{H}$. Denote by $\mathcal{F}$ the unit ball $\mathcal{F} = \{ h \in \mathcal{H} : \| h \|_{\mathcal{H}} \leq 1 \}$.

For a distribution $F$ taking values in $\Omega$ the map $\mu[F]$ defined by

$$\mu[F] := \int_{\Omega} \kappa(\omega, \cdot) \, dF(\omega).$$

belongs to $\mathcal{H}$. If $\kappa$ is a universal kernel, then $\mu$ is an injective map.

Let $F$ and $G$ be probability distributions taking values in $\Omega$; $X, X' \sim F$ and $Y, Y' \sim G$. Then

$$\| \mu[F] - \mu[G] \|^2_{\mathcal{H}} = \sup_{h \in \mathcal{F}} \left[ \mathbb{E}_F[h] - \mathbb{E}_G[h] \right]^2$$

$$= \mathbb{E}[\kappa(X, X')] - 2\mathbb{E}[\kappa(X, Y)] + \mathbb{E}[\kappa(Y, Y')].$$

(2)

is an integral probability metric, termed the maximum mean discrepancy

Gretton et al. (2012).
Denote by $\Phi: \Omega \mapsto \mathcal{H}$ the canonical feature map

$$\Phi(X) = \kappa(\cdot, X)$$

of $\kappa$. Given $\{X_i\} \overset{\text{i.i.d}}{\sim} F$ and $\{Y_i\} \overset{\text{i.i.d}}{\sim} G$, the quantity $V_{n,m}(X, Y)$

$$V_{n,m}(X, Y) = \left\| \frac{1}{n} \sum_{i=1}^{n} \Phi(X_i) - \frac{1}{m} \sum_{k=1}^{n} \Phi(Y_k) \right\|_{\mathcal{H}}^2$$

$$= \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \kappa(X_i, X_j) - \frac{2}{mn} \sum_{i=1}^{m} \sum_{k=1}^{n} \kappa(X_i, Y_k)$$

$$+ \frac{1}{m^2} \sum_{k=1}^{m} \sum_{l=1}^{m} \kappa(Y_k, Y_l).$$

is a consistent estimate of $\| \mu[F] - \mu[G] \|_{\mathcal{H}}^2$. 
Denote by $\hat{X} = \{\hat{X}_1, \ldots, \hat{X}_n\}$ and $\hat{Y} = \{\hat{Y}_1, \ldots, \hat{Y}_m\}$ the adjacency spectral embedding of $A$ and $B$, respectively. Assume that $\kappa$ is a unitarily invariant kernel, e.g., a radial kernel. Define the test statistic $V_{n,m}(\hat{X}, \hat{Y})$ as follows:

$$V_{n,m}(\hat{X}, \hat{Y}) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \kappa(\hat{X}_i, \hat{X}_j) - \frac{2}{mn} \sum_{i=1}^{n} \sum_{k=1}^{m} \kappa(\hat{X}_i, \hat{Y}_k) + \frac{1}{m^2} \sum_{l=1}^{m} \sum_{k=1}^{m} \kappa(\hat{Y}_k, \hat{Y}_l)$$
Let \((X, A) \sim \text{RDPG}(F)\) and \((Y, B) \sim \text{RDPG}(G)\) be independent random dot product graphs with latent position distributions \(F\) and \(G\) satisfying distinct eigenvalues assumption. Consider the hypothesis test

\[
\mathcal{H}_0: F =_W G \quad \text{against} \quad \mathcal{H}_1: F \neq_W G
\]

Suppose \(m, n \to \infty\) and \(m/(m+n) \to \rho \in (0, 1)\). Then under the null

\[
(m + n)(V_{n,m}(\hat{X}, \hat{Y}) - V_{n,m}(X, YW)) \xrightarrow{a.s.} 0
\]

where \(W\) is any orthogonal matrix such that \(F = G \circ W\).
Eq. (3) that

\[(m + n)(V_{n,m}(\hat{X}, \hat{Y}) - V_{n,m}(X, YW)) \xrightarrow{\text{a.s.}} 0\]

follows from the following bound

\[
\sup_{f \in \mathcal{F}} \left| \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (f(W \hat{X}_i) - f(X_i)) \right| \xrightarrow{\text{a.s.}} 0
\]

established via Taylor’s expansion and a covering number argument.
Limiting distribution of $V_{n,m}(\hat{X}, \hat{Y})$.

Hence under the null hypothesis of $F =_W G$, evoking previous results of Anderson et al. (1994) and Gretton et al. (2012) for $V_{n,m}(X, Y)$, one has

$$(m + n)V_{n,m}(\hat{X}, \hat{Y}) \xrightarrow{d} \frac{1}{\rho(1 - \rho)} \sum_{l=1}^{\infty} \lambda_l \chi_{1l}^2$$

(4)

where $\{\chi_{1l}^2\}$ are independent $\chi^2$ random variables with one degree of freedom and $\{\lambda_l\}$ are the eigenvalues of the integral operator

$$I_{F, \tilde{\kappa}}(\phi) = \int_{\Omega} \phi(y)\tilde{\kappa}(x, y)dF(y)$$
Figure 1: Distribution of test statistics under null and alternative as computed from the latent positions and those estimated from adjacency spectral embedding for testing the null hypothesis $F = W G$. 
\[ \epsilon = 0.02 \quad \epsilon = 0.05 \quad \epsilon = 0.1 \]

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**Table 1**: Power estimates for testing the null hypothesis \( F =_W G \) at a significance level of \( \alpha = 0.05 \) using bootstrap permutation tests for \( V_{n,m}(\hat{X}, \hat{Y}) \) and \( V_{n,m}(X, Y) \). In each bootstrap test, \( B = 200 \) bootstrap samples were generated. Each estimate of power is based on 1000 Monte Carlo replicates of the corresponding bootstrap test.


