Estimation of the Sample Fréchet Mean: 
A Convolutional Neural Network Approach

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Abstract

This work aims to address this rising demand for novel tools in statistical 
and machine learning for “graph-valued random variables” by proposing 
a fast algorithm to compute the sample Fréchet mean, which replaces 
The concept of sample mean for graphs (or networks). We use convolutional 
neural networks to learn the morphology of the graphs in a set of 
graphs. Our experiments on several ensembles of random graphs demonstrate that our method can reliably recover the sample Fréchet mean.

Keywords: Fréchet mean graph, convolutional neural networks, statistical 
network analysis

1 Introduction

The purpose of this paper is to present a fast method to compute the sample 
Fréchet mean graph using convolutional neural networks. The Fréchet mean 
(or median) graph, which extends the notion of mean to probability measures 
defined on metric spaces (Fréchet, 1947), has become a standard tool for the 
analysis of graph-valued data (e.g., (Dubey and Müller, 2020; Ferrer et al, 
2010; Ginestet et al, 2017; Jain, 2016b; Josephs et al, 2021; Kolaczyk et al, 
2020; Lunagómez et al, 2020) and references therein). The vital role played 
by the Fréchet mean as a location parameter (Jain and Obermayer, 2012; 
Jain, 2016a; Kolaczyk et al, 2020), is exemplified in the works of (Banks and 
Constantine, 1998; Lunagómez et al, 2020), who have created novel families
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1.1 Related work

The Fréchet mean graph has been studied in the context where the distance that is used to compare graphs is the edit distance (e.g., (Bardaji et al, 2010b,a; Ginestet, 2012; Jain and Obermayer, 2009; Jiang et al, 2001) and references therein), the Frobenius distance (e.g., (Boria et al, 2020; Jain and Obermayer, 2008; Kolouri et al, 2021) and references therein), and the Gromov-Wasserstein distance (e.g., (Barbe et al, 2020; Chowdhury and Mémoli, 2019; Gu et al, 2015; Heinemann et al, 2022; Métivier et al, 2019; Vayer et al, 2020) and references therein). In this paper, we propose to compare graphs using the eigenvalues of their respective adjacency matrices.

The Fréchet mean graph is the solution to a minimization problem that is intractable for most distances (e.g., (Anderes et al, 2016; Bardaji et al, 2010b; Heinemann et al, 2022; Jain and Obermayer, 2009; Patterson, 2021) and references therein). For this reason several alternatives have been proposed to solve the minimization problem (2). A popular approach consists in embedding the graphs in a Euclidean space, wherein one can trivially find the mean of the set (e.g., (Ferrer et al, 2010; Kolouri et al, 2021; Simou et al, 2020) and references therein). Several researchers have proposed recently to learn the embedding from massive datasets of existing networks. Such algorithms learn an embedding (e.g., (Preuer et al, 2018) and references therein) from a set of graphs into Euclidean space, and then compute a notion of similarity between the embedded graphs. Several authors have proposed to use convolutional neural networks to compute the intractable Wasserstein distance (e.g., (Brogat-Motte et al, 2022; Solomon et al, 2015) and references therein).

When the graphs \( \{G^{(k)}\}_{1 \leq k \leq N} \), in the sample are not defined on the same vertex set, then one needs to solve a graph isomorphism problem to jointly align the graphs (e.g., (Ferrer et al, 2010) and references therein). In this paper, we assume that the graphs are defined on the same vertex set, and we avoid the added combinatorial complexity associated with the graph alignment problem.

1.2 The Fréchet mean graph

Let \( \mathcal{G} \) be the set of all simple labeled graphs with vertex set \( \{1, \ldots, n\} \), and let \( S \) be the set of \( n \times n \) adjacency matrices of graphs in \( \mathcal{G} \),

\[
S = \{ A \in \{0, 1\}^{n \times n}; \text{ where } a_{ij} = a_{ji}, \text{ and } a_{i,i} = 0; \ 1 \leq i < j \leq n \}. \tag{1}
\]

We equip \( \mathcal{G} \) with a metric \( d \) to measure the distance between two graphs. We characterize the “average” of a sample of graphs \( \{G^{(1)}, \ldots, G^{(N)}\} \), which are defined on the same vertex set \( \{1, \ldots, n\} \), with the sample Fréchet mean graphs (Fréchet, 1947).
Definition 1 The sample Fréchet mean graphs are solutions to

\[ \hat{\mu}_N[G] = \arg\min_{G \in \mathcal{G}} \frac{1}{N} \sum_{k=1}^{N} d^2(G, G^{(k)}). \]  

Solutions to the minimization problem (2) always exist, but the minimizers need not be unique. All our results are stated in terms of any of the elements in the set of minimizers of (2). To simplify the exposition, we refer to the sample Fréchet mean graph as any representative element of the class of solutions to (2), and with a slight abuse of notation (which is commonly used), we denote by \( \hat{\mu}_N[G] \) this representative element.

1.3 Our main contributions

In this paper, we propose a novel method for calculating the sample Fréchet mean \( \hat{\mu}_N[G] \). Our line of attack relies on the following key ideas: (1) stochastic block models with community of various sizes provide universal approximants to graphs (Bickel and Chen, 2009; Ferguson and Meyer, 2022c; Olhede and Wolfe, 2014), (2) computing the sample Fréchet mean of stochastic block models (sampled from the same probability measure) can be performed using simple averaging and nonlinear thresholding (Meyer, 2022). We propose therefore to combine these two principles within a convolutional network, which learns the combined optimal (stochastic block model) approximation of the graphs in a sample, together with the averaging and nonlinear thresholding that yields the sample Fréchet mean.

We show in many experiments with various ensembles of random graphs, that the estimate of the Fréchet mean computed with our method is very close to the true Fréchet mean (computed using a brute force approach) when the distance used to compare graphs is the adjacency spectral pseudo-distance. This property is a consequence of the following fact: the stochastic block model that provides a nonlinear approximation to all the graphs in the sample is able to capture the large scale connectivity features of the Fréchet mean graph. Conversely, we also show that the local connectivity structure (as quantified by the degree distribution) of the true Fréchet mean is very similar to the corresponding connectivity structure of the graph computed with our method.

This experimental result is significant because the convolutional neural network does not require the computational costly computation of the eigenvalues of the graphs in the sample.

1.4 Organization of the paper

In the next section, we introduce the main concepts and associated notations. In section 3, we provide an overview of our approach. The architecture of the convolutional neural network is described in section 4. The random graph ensembles that are used to train the convolutional neural network are presented in section 5. In the same section, we describe the training procedure. Results of
experiments conducted on several ensembles of random graphs are presented in section 6. All relevant code, including the pre-trained models, is available at (Sanchez, 2022).

2 Preliminary and Notations

For a graph $G \in \mathcal{G}$, we denote by $A$ its adjacency matrix. We define the degree of a vertex, $i \in V$ as $d_i = \sum_{i \sim j} 1$. The degree matrix, $D$, of graph $G$ is the diagonal matrix defined by

$$D = \text{diag}(d_1, \ldots, d_n)$$  \hspace{1cm} (3)

and the combinatorial Laplacian matrix, $L$, is defined by

$$L = D - A, \hspace{1cm} (4)$$

where $I$ is the $n \times n$ identity matrix.

**Definition 2** We denote by $\lambda(A) = [\lambda_1(A) \cdots \lambda_n(A)]$, the vector of sorted eigenvalues of the adjacency matrix $A$, with the convention that $\lambda_1(A) \geq \ldots \geq \lambda_n(A)$.

Similarly, we denote by $\lambda(L)$ the vector of sorted eigenvalues in ascending order of the normalized Laplacian matrix $L$, with the convention that $\lambda_1(L) \leq \ldots \leq \lambda_n(L)$.

2.1 Distances between graphs

In this work, we propose an algorithm to construct the barycenter of a sample of graphs. The notion of barycenter, or Fréchet mean, requires that we define a distance on the set of graphs. The distance quantifies our notion of similarity between graphs. To simplify the exposition, we only consider graphs defined on the same vertex set. In practice, one often needs to compare graphs of different sizes. Because we use spectral distances, we can easily extend theoretically and numerically these distances to graphs of different sizes, without having to solve the graph isomorphism problem (McKay and Piperno, 2014).

We recognize that the computation of the sample Fréchet mean requires that the distance $d$ being used in (2) be adapted to the distinctive characteristics (e.g., degree distribution, presence of communities, hubs, connectivity structure, etc.) of the sample of graphs. In the absence of a universal distance that would be optimal for all graphs (Donnat and Holmes, 2018; Wills and Meyer, 2020), we propose instead to adapt the distance to the characteristic features of the graph ensembles from which the sample is drawn (Donnat and Holmes, 2018; Wills and Meyer, 2020).

The authors in (Wills and Meyer, 2020) provide a comprehensive analysis of the properties of many graph distances in the context of graph valued machine
learning algorithms. They show that the adjacency spectral pseudo-distance (5) defined as follows,

**Definition 3** Let $G, G' \in \mathcal{G}$ be two graphs with adjacency matrix $A$ and $A'$ respectively. We define the adjacency spectral pseudometric as the $\ell_2$ norm between the vectors of eigenvalues $\lambda(A)$ and $\lambda(A')$ of $A$ and $A'$ respectively,

$$d_A(G, G') = \|\lambda(A) - \lambda(A')\|_2.$$  

(5)

provides the largest decision boundaries between a class of stochastic block model graphs and a class of Erdős-Rényi random graphs. We adopt the adjacency spectral pseudo-distance to quantify the variations within the ensemble of stochastic block models.

Conversely, the combinatorial Laplacian spectral pseudo-metric, defined by

**Definition 4** Let $G, G' \in \mathcal{G}$ with combinatorial Laplacian matrix $L$ and $L'$ respectively. We define the combinatorial Laplacian spectral pseudometric as the $\ell_2$ norm between the vectors of eigenvalues $\lambda(L)$ and $\lambda(L')$ of $L$ and $L'$ respectively,

$$d_L(G, G') = \|\lambda(L) - \lambda(L')\|_2.$$  

(6)

was shown in (Wills and Meyer, 2020) to provide the largest margin when comparing a class of preferential attachment graphs (Barabási and Albert, 1999) and a class of random graphs. For this reason, we use the Laplacian spectral pseudo-distance to quantify the variations within the ensemble of preferential attachment graphs.

We note that $d_A$ and $d_L$ are only a pseudo-distance: they satisfy the symmetry and triangle inequality axioms, but not the identity axiom. Instead, the pseudo-distances satisfy the reflexivity axiom, $\forall G \in \mathcal{G}, d_A(G, G) = d_L(G, G) = 0$. However, an advantage of these pseudo-distances is that they do not require node correspondence between $G$ and $G'$.

Finally, when comparing inhomogeneous Erdős-Rényi random graphs, we use the Hamming distance, $d_H$, defined as follows.

**Definition 5** The Hamming distance between $G$ and $G'$ with adjacency matrix $A$ and $A'$ respectively, is given by

$$d_H(G, G') = \sum_{1 \leq i < j \leq n} |a_{ij} - a'_{ij}|.$$  

(7)

The advantage of the Hamming distance is that the population and sample Fréchet means can be computed in closed form (Meyer, 2022).
2.2 The sample Fréchet mean, our estimate of the Fréchet mean, and the sample mean adjacency matrix

Let \( \{G^{(k)}\}_{1 \leq k \leq N} \), be a set of \( N \) graphs. We recall and introduce some notations associated with the computation of the sample Fréchet mean graph. In the following we need to compute (using a brute force approach) the true Fréchet mean, \( \hat{\mu}_N[G] \), solution to the discrete optimization problem (2).

**Definition 6** When optimizing the convolutional neural network, in section 4, we call the adjacency matrix of the true Fréchet mean graph, \( \hat{\mu}_N[A] \), the target adjacency matrix.

In contrast, we denote by \( \mu^*_N[G] \) the estimate of the sample Fréchet mean graph computed using the method described in this paper, and outlined in the next section. The corresponding adjacency matrix is denoted by \( \mu^*_N[A] \).

We denote by \( \hat{E}[A] \) the sample mean adjacency matrix

\[
\hat{E}[A] = \frac{1}{N} \sum_{k=1}^{N} A^{(k)}. \tag{8}
\]

The sample mean matrix is the input to the convolutional neural network.

Finally, we define the the naive sample Fréchet mean, \( \tilde{\mu}_N \), to be the thresholded sample mean adjacency matrix,

\[
[\tilde{\mu}_N]_{ij} = \begin{cases} 
1 & \text{if } \hat{E}[A]_{ij} > 1/2, \\
0 & \text{otherwise}. 
\end{cases} \tag{9}
\]

Our goal is to demonstrate that \( \mu^*_N[A] \) is close to the true sample Fréchet mean, \( \hat{\mu}_N[A] \). In order to provide a reasonable upper bound on the approximation error between the different models and the true sample Fréchet mean, we define the concept of “naive sample Fréchet mean”. The naive sample mean Fréchet mean, \( \tilde{\mu}_N \), only provides a poor man’s estimate of sample Fréchet mean. Interestingly, the naive sample Fréchet mean \( \tilde{\mu}_N \) coincides with the true sample Fréchet mean \( \hat{\mu}_N \) when the graphs in the ensemble have a reasonably simple geometry (Meyer, 2021), for instance when all the graphs in the sample are generated from an inhomogeneous Erdős-Rényi random graph model.

3 Overview of our method

3.1 Computing an approximation to the sample Fréchet mean

The optimization problem (2) is non convex, and in general the computation of the Fréchet mean is NP-complete. In this work, we propose a fast method to compute an approximation to the sample Fréchet mean of a set of \( N \) graphs \( \{G^{(k)}\}_{1 \leq k \leq N} \). Our line of attack relies on the idea of replacing the
intractable problem (2) with the estimation of a parametric graph model that approximates the sample Fréchet mean, \( \hat{\mu}_N[A] \), arbitrarily well.

The ensemble of stochastic block models, \( SBM \), with community of various sizes, is a family of parametric model that provides universal approximants to graphs (Ferguson and Meyer, 2022c; Olhede and Wolfe, 2014). This approximation property of the stochastic block model holds for various norms: the \( \ell^2 \) difference between the corresponding spectra (Ferguson and Meyer, 2022c,a), or the \( L^2 \) difference between the corresponding graphons (Olhede and Wolfe, 2014; Wolfe and Olhede, 2013). Different algorithms have been proposed to compute the optimal stochastic block model approximation to a graph (Ferguson and Meyer, 2022c; Olhede and Wolfe, 2014; Wolfe and Olhede, 2013).

We propose therefore to estimate the SBM graph, \( SBM(P) \), with edge probability matrix \( P \), whose population Fréchet mean \( \mu[P] \), is as close as possible to the sample Fréchet mean \( \hat{\mu}_N[A] \). We replace (2) with the following optimization program,

\[
\min_{SBM(P) \in SBM} d_A(\hat{\mu}_N[A], \mu[P]), \tag{10}
\]

where \( d_A \) is the adjacency spectral pseudometric (5), and \( SBM \) is the set of adjacency matrices of the stochastic block models. We use the adjacency spectral pseudometric, because we know from (Ferguson and Meyer, 2022c,a) that we can make this distance in (10) asymptotically small in the limit of large graph sizes.

Each stochastic block model \( SBM(P) \in SBM \) is a random graph of size \( n \) with edge probability matrix \( P \) (Abbe, 2018). The set \( SBM \) is therefore parameterized by the set of \( n \times n \) edge probability matrices \( P \).

To solve (10), we first replace the population Fréchet mean \( \mu[P] \) of \( SBM(P) \) with the sample Fréchet mean, \( \hat{\mu}_N[B] \), computed from a sample of adjacency matrices \( B^{(k)} \) sampled from the stochastic block models \( SBM(P) \).

This approximation is justified by the fact that the sample Fréchet mean, \( \hat{\mu}_N[B] \), converges in probability to the corresponding population Fréchet mean, \( \mu[P] \), in the limit of large graph sizes \( (n \to \infty) \) (Meyer, 2022). The problem (10) is therefore replaced by

\[
\min_{SBM(P) \in SBM} d_A(\hat{\mu}_N[A], \hat{\mu}_N[B]), \quad \text{where } B \sim SBM(P). \tag{11}
\]

Finally, we take advantage of the following property: the sample Fréchet mean (computed using the Hamming distance) of a sample of stochastic block models \( B \sim SBM(P) \) is obtained by thresholding the sample mean adjacency matrix \( \hat{E}[B] \) (Meyer, 2022). In other words,

\[
[\hat{\mu}_N[B]]_{ij} = \left\{ \begin{array}{ll} 1 & \text{if } \hat{E}[B]_{ij} > 1/2, \\ 0 & \text{otherwise.} \end{array} \right. \tag{12}
\]
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We note that this simple computation of the sample Fréchet mean does not hold for the adjacency spectral pseudo-distance, $d_A$. Notwithstanding our choice of distance, and inspired by the nonlinear rule (12), we propose instead to replace $\hat{E}[B]$ with $\hat{E}[A]$, the sample mean adjacency matrix of the sample $\{A^{(k)}\}, k = 1, \ldots, N$, and to replace the nonlinear thresholding matrix function $\tau$ in (12) with a more general nonlinear matrix function $\Phi$. We therefore consider the following optimization program,

$$\min_{\Phi} d_H(\hat{\mu}_N[A], \Phi(\hat{E}[A])), \tag{13}$$

where $\Phi$ is a nonlinear matrix function that operates on the entries of the matrix $\hat{E}[A]$. The matrix function $\Phi$ needs to account for the thresholding $\tau$ introduced in (12), but may also account for the approximation errors introduced by replacing the optimization program (2) with the program (13).

In the next section, we explain how we can learn the matrix function $\Phi$, which maps the sample mean adjacency matrix to the sample Fréchet mean, using a convolutional neural network.

### 3.2 Learning the nonlinear matrix function $\Phi$

We propose to use a convolutional network (described in detail in section 4) to learn the combined optimal approximation of the graphs in a sample along with the averaging and nonlinear thresholding that yields the Fréchet mean. The core engine of the nonlinear matrix function $\Phi$ is a clustering (segmentation) algorithm that partitions the sample mean adjacency matrix into modules or communities. Communities are formed by regions wherein the nodes are densely connected; whereas the other regions correspond to “non-edge” entries of the adjacency matrix. The sample mean average adjacency matrix can be interpreted as a weighted graph; the outcome of the partitioning is an unweighted graph.

Our approach is similar to the sorting and smoothing approach of the authors in (Chan and Airoldi, 2014) who use Total Variation (TV) denoising to segment the image formed by the adjacency matrix (re-ordered according to the degree of each node). The authors in (Wei et al, 2018; Wei, 2021) also use image segmentation to estimate the graphon that is used to generate an observed adjacency matrix. A clustering algorithm is also used by the authors in (Cai et al, 2015) to estimate a step graphon.

Fig. 1 provides a visual example of the input sample mean adjacency matrix, $\hat{E}[A]$ (top-left), the true sample Fréchet mean graph’s adjacency matrix, $\hat{\mu}_N[A]$ (bottom-left), and the estimate of the Fréchet mean using our approach, $\mu^*_N[G]$ (bottom-right).

### 4 Convolutional Neural Network Framework

The input to the convolutional neural network is the sample mean adjacency matrix, $\hat{E}[A]$, and the output is $\mu^*_N[G]$. During the training phase, the
neural network is provided with the true sample Fréchet mean, $\hat{\mu}_N[A]$. The true Fréchet mean is computed using a brute force search over the space of undirected unweighted graphs, $\mathcal{G}$.

When computing $\hat{\mu}_N[A]$ during the training or evaluation of the algorithm on a specific graph ensemble, we use the metric that is best adapted to this ensemble: the Hamming distance $d_H$ for inhomogeneous Erdős-Rényi random graphs, the adjacency spectral pseudo-distance $d_A$ for stochastic block-models, and the Laplacian spectral pseudo-distance $d_L$ for preferential attachment graphs.

The parameters of the network are then optimized in order to learn the nonlinear map $\Phi$ that computes $\hat{\mu}_N[A]$ when presented with the input $\hat{E}[A]$

The design of the architecture of the convolutional neural network relies on the simple idea that $\Phi$, defined in the program (13), should be able to perform an entry-wise thresholding of the sample mean adjacency matrix $\hat{E}[A]$, defined in (12), when the input graphs are realizations of inhomogeneous Erdős-Rényi random graphs (with the same edge probability matrix $P$). We propose to model this nonlinear transformation with a segmentation algorithm that partitions the sample mean adjacency matrix into modules of densely connected vertices.

4.1 U-Nets

Given the important role segmentation plays in many fields, it is not surprising that there has been many works dedicated to its advancement. Undoubtedly,
the U-Net algorithm (Ronneberger et al., 2015) has been proven as a key staple in the field. U-Net is a CNN architecture composed of encoder and decoder structures each with convolutional/down-sampling and deconvolutional/up-sampling stages. Each of the convolutional stages are comprised of two $3 \times 3$ unpadded convolutions followed by a rectified linear unit (ReLU) and a $2 \times 2$ max pooling operation. At each down-sampling stage, the number of feature channels are doubled. At each of the up-sampling stages, an up-sampling of the feature map followed by a $2$ convolution occurs, halving the number of feature channels. A concatenation with the corresponding deconvolutional stage is done, followed by two $3 \times 3$ convolutions and a ReLU. A final $1 \times 1$ convolution is done in order to achieve the desired output size.

Our model follows an architecture very similar to U-Net and is depicted in Fig. 2. We have a set of 2 down-sampling stages coupled with 2 up-sampling stages, each of which are comprised of $3 \times 3$ convolutions and ReLU activation. Again, borrowing from U-Net, we add cross concatenations from the down-sampling stages to their corresponding up-sampling stage. We then perform a final $1 \times 1$ convolution with a sigmoid activation to achieve our desired output shape.

Fig. 2 Our model architecture corresponding to a $28 \times 28 \times 1$ input tensor. Each blue box corresponds to a multi-channel feature map. The x-y dimensions are given in the lower left of each box. The number of features is given by the number above each box. The arrows represent the different operations.
5 Data Sets and Training

As mentioned above, we restrict ourselves to undirected and unweighted graphs with \( n = 28 \) nodes. We restrict ourselves to graphs of such small size because our interest is to demonstrate the feasibility of our approach, and therefore we need to compute the true sample Fréchet mean graph, solution of (2). This optimization problem is solved using an exhaustive search, which is very demanding and unrealistic for large graphs. The computational cost scales with the sample size, and we therefore restrict ourselves to a sample size of \( N = 10 \).

We plan to extend our implementation to larger graphs and larger sample size in the future. We note that others have also evaluated graph-valued machine learning algorithms on graphs of small size (e.g., size of the benchmark graphs for the comparison and evaluation of graph-valued algorithms (Morris et al, 2020)).

Our code, including the pre-trained models, is available (Sanchez, 2022).

We consider three distinct ensemble of random graphs in order to generate both our training and testing data: inhomogeneous Erdős-Rényi random graphs, the stochastic block model, and the Barabasi-Albert preferential attachment model. We consider existing ensembles of random graphs as prototypical examples of certain graph structures, which are the building blocks of existing real world networks. Our investigation is concerned with the relationship between the families of graph ensembles and the ability of one ensemble to provide the best training dataset for the other ensembles. We expect that the differences between the structural features characteristic of these ensembles affect the outcome of the training and the subsequent performance of the algorithm.

For each ensemble of random graphs, we generate a training set of \( m = 3,600 \) graphs from that ensemble. The training sample is then divided into batches of size \( N = 10 \). For each batch, we compute the exact sample Fréchet mean graph, \( \hat{\mu}_N[A] \), solution to (2), and the sample mean adjacency matrix of the \( N \) adjacency matrices, \( \hat{E}_N[A] \).

5.1 Inhomogeneous Erdős-Rényi Graphs

We first consider the probability space \( \mathcal{G}(n, P) \) formed by inhomogeneous Erdős-Rényi random graphs (Bollobás et al, 2007), defined on the vertex set \( \{1, \ldots, n\} \), where a graph \( G \) with adjacency matrix \( A \) has probability,

\[
\mathbb{P}(A) = \prod_{1 \leq i < j \leq n} [p_{ij}]^{a_{ij}} [1 - p_{ij}]^{1 - a_{ij}}.
\]

The \( n \times n \) matrix \( P = [p_{ij}] \) determines the edge probabilities \( 0 \leq p_{ij} \leq 1 \), with \( p_{ii} = 0 \). In the case of a sample of inhomogeneous Erdős-Rényi random graphs, all generated from the same probability matrix \( P \), one can easily compute the sample Fréchet mean graph, \( \hat{\mu}_N[G] \). Indeed, the adjacency matrix \( \hat{\mu}_N[A] \) of
Algorithm 1 Inhomogeneous Erdős-Rényi Training Data Generation

for i in 1:36 do
    a = uniform(0.5,5)
    b = uniform(0.5,5)
    for j in 1:100 do
        $P = \text{Beta}(a,b)$
        for k in 1:10 do
            sample[k] = E.R.($P$)
        end for
        $A_I = \sum_{1}^{10} \text{sample}$
        $\hat{E}[A] = \text{KnownMean}(P)$
    end for
    InputList.append($A_I$)
    TargetList.append($\hat{E}[A]$)
end for

$\mu_N[\mathcal{G}]$ is given by (Meyer, 2021)

$$\hat{\mu}_N[A]_{ij} = \begin{cases} 1 & \hat{E}[A]_{ij} > \frac{1}{2}, \\ 0 & \text{otherwise.} \end{cases} \quad (15)$$

We varied the edge probability matrix, $P$. For each simulation, $P$ was chosen randomly using independent (up to symmetry) beta random variables, $p_{ij} \sim \text{beta}(a,b)$. The parameters $a$ and $b$ were sampled uniformly on [0, 5]. Alg. 1 provides a description of this process.

5.2 Stochastic Block Model

One important property of real world networks is community structure. Vertices form densely connected communities, with the connection between communities being sparse, or non-existent. This motivates the use of the stochastic blockmodel. In this model, the vertex set can be partitioned into non-overlapping sets referred to as “communities”. Each edge $e = (i, j)$ exists independently with probability $p$ if $i$ and $j$ are in the same community, and $q$ if $i$ and $j$ are in distinct communities.

The training dataset is formed of $m/2$ graph with two communities of size $n/2 = 14$, and $m/2$ graphs with three communities with sizes 10, 10, and 8. We then sample the edge probabilities, $p$ and $q$ uniformly on [0.5, 0.9] and on [0.1, 0.5] respectively. We restrict our samples to only connected graphs. Alg. 2 provides a description of this process.
Algorithm 2 Stochastic Block Model Training Data Generation

Require: BlockSize2 = [14, 14]
Require: BlockSize3 = [10, 10, 8]

for i in 1:36 do
    p = uniform(0.5, 0.9)
    q = uniform(0.01, 0.5)
    if i < 19 then
        for j in 1:100 do
            for k in 1:10 do
                $A[k] = S.B.(p, q, \text{BlockSize2})$
            end for
            $A_I = \sum_{k=1}^{10} A$
            $\hat{E}[A] = \text{argmin}_{G \in A} \frac{1}{10} \sum_{k=1}^{10} d^2_A(G, G^{(k)})$
        end for
    else if i ≥ 19 then
        for j in 1:100 do
            for k in 1:10 do
                $A[k] = S.B.(p, q, \text{BlockSize3})$
            end for
            $A_I = \sum_{k=1}^{10} A$
            $\hat{E}[A] = \text{argmin}_{G \in A} \frac{1}{10} \sum_{k=1}^{10} d^2_A(G, G^{(k)})$
        end for
    end if
    InputList.append($A_I$)
    TargetList.append($\hat{E}[A]$)
end for

5.3 Preferential Attachment Graphs

Another frequently studied feature for real-world graphs is the degree distribution. Real-world graphs, such as social and computer networks, have a power-law tail, $P(d) \propto d^{-\gamma}$ where $\gamma \in [2, 3]$. These distributions are referred to as “scale-free” (Barabási and Albert, 1999).

The preferential attachment model is a random graph model that fits the characteristics of “scale-free”. The model has two parameters, $l$ (density of the graph) and $n$ (size of the graph). We begin by initializing a star graph with $l + 1$ vertices, with vertex $l + 1$ having degree $l$ and all others having degree 1. Then, for each $l + 1 < i \leq n$, we add a vertex, and randomly attach it to $l$ vertices already present in the graph, where the probability of $i$ attaching to $v$ is proportional to the degree of $v$. We stop once the graph contains $n$ vertices.

The training set includes $m$ graphs for a variety of $l$ values (see Alg. 3).
Algorithm 3 Preferential Attachment Data Generation

Require: \( l = [5, 7, 10, 12, 15, 17, 20, 22, 25] \)

for \( i \in l \) do
  for \( j \) in 1:400 do
    for \( k \) in 1:10 do
      \( A[k] = P.A.(l, n=28) \)
    end for
    \( A_I = \sum_{1}^{10} A \)
    \( \hat{E}[A] = \arg\min_{G \in A} \frac{1}{10} \sum_{k=1}^{10} d^2_G(G, G^{(k)}) \)
  end for
  InputList.append(\( A_I \))
  TargetList.append(\( \hat{E}[A] \))
end for

5.4 Training

We train four distinct versions of the same exact model described in Section 4 using four different training sets. We call each version of the algorithm with a different name that encodes the name of the graph ensembles used to train the model: IER-Unet, SBM-Unet, BA-Unet. We also consider a model, Gen-Unet, that is trained using a training set formed by the union of the three previous training sets.

We employ batch Adam optimization coupled with a binary cross entropy as our loss in order to train our models. Binary cross entropy is a natural choice for our loss function as it is widely used in binary classification tasks. We refer the reader to (Kingma and Ba, 2015) for more details pertaining to Adam.

6 Experiments

We validate our approach with a wide variety of experiments using the three random graph ensembles. For each experiment, we report several statistics that characterize the precision of our estimate of the sample Fréchet mean graph.

Our test data is composed of \( l = 3 \times 900 \) adjacency matrices from each of the three random graph ensembles: Erdős-Rényi, stochastic block model, and preferential attachment. In the next section, we describe the methodology that we use to quantify the results of the experiments.

6.1 Evaluation protocol

In the following, we describe the gauges that we use to quantify the error between the true and the estimated sample Fréchet mean graph. Our comparison combines two different scales: the large to medium scale connectivity quantified by the largest eigenvalues of the adjacency matrix, and the fine scale connectivity, formed by the ego-net quantified by the degree distribution.
The spectral differences.

**Definition 7** Given a sample of $N$ adjacency matrices, $A_1, \ldots, A_N$, and their vectors of ordered eigenvalues (see Def. 2), $\lambda(A_1), \ldots, \lambda(A_N)$, the sample mean vector of eigenvalues is given by,

$$\hat{E}[\lambda] = \frac{1}{N} \sum_{k=1}^{N} \lambda(A_k).$$

(16)

We define the vector of eigenvalues of the sample Fréchet mean as follows,

$$\lambda(\hat{\mu}_N) = \lambda(\hat{\mu}_N[A]).$$

(17)

Finally, we denote by $\lambda(\mu^*_N)$, the spectrum of our estimate, $\mu^*_N[A]$ of the sample Fréchet mean,

$$\lambda(\mu^*_N) = \lambda(\mu^*_N[A]).$$

(18)

To simplify the exposition, and alleviate the complexity of the notations, we remove the notation $[A]$ in $\hat{E}[\lambda], \lambda(\hat{\mu}_N), \text{and } \lambda(\mu^*_N)$, which indicate the dependency of the sample mean on the adjacency matrices in the sample, $A_1, \ldots, A_N$.

We expect that $\hat{E}[\lambda]$ be close to $\lambda(\hat{\mu}_N)$, since as shown in (Ferguson and Meyer, 2022b), the sample mean spectrum is asymptotically close to the spectrum of the sample Fréchet mean, in the limit of large graph size. In order to compare $\lambda(\hat{\mu}_N)$ and our estimate $\lambda(\mu^*_N)$, we define the vector of absolute differences ($\Delta \lambda$).

**Definition 8** Let $A_1$ and $A_2$ be the adjacency matrices of two graphs. Let $\lambda(A_1)$ and $\lambda(A_2)$ be their respective eigenvalues vectors (with entries sorted by their magnitude). We denote by

$$\Delta \lambda(A_1, A_2) = [|\lambda_1(A_1) - \lambda_1(A_2)| \ldots |\lambda_n(A_1) - \lambda_n(A_2)|] ,$$

(19)

the vector of absolute differences between the eigenvalues of $A_1$ and $A_2$.

Because the eigenvalues of the adjacency matrix are not normalized, we introduce the vector of relative difference between two vectors of eigenvalues with the following definition.

**Definition 9** Let $A_1$ and $A_2$ be the adjacency matrices of two graphs. Let $\lambda(A_1)$ and $\lambda(A_2)$ be their respective eigenvalues vectors (with entries sorted by their magnitude). We denote by

$$\Delta^p \lambda(A_1, A_2) = \left[ \frac{|\lambda_1(A_1) - \lambda_1(A_2)|}{|\lambda_1(A_2)|} \ldots \frac{|\lambda_n(A_1) - \lambda_n(A_2)|}{|\lambda_1(A_2)|} \right] ,$$

(20)

the vector of relative difference per eigenvalue.

In this paper, we are concerned with the comparison of the eigenvalues of $\mu^*_N[A]$ and these of $\hat{\mu}_N[A]$. We compute the vectors of (absolute and relative) differences, $\Delta$ and $\Delta^p$. In order to alleviate the complexity of the notations, we
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remove the notation $[A]$, which indicate the dependency of the sample mean on the adjacency matrices in the sample, $A_1, \ldots, A_N$, in these differences. We therefore define,

$$\Delta_\lambda(\hat{\mu}_N, \mu^*_N) \overset{\text{def}}{=} \Delta_\lambda(\hat{\mu}_N[A], \mu^*_N[A]) \quad \text{and} \quad \Delta_\lambda^p(\hat{\mu}_N, \mu^*_N) \overset{\text{def}}{=} \Delta_\lambda^p(\hat{\mu}_N[A], \mu^*_N[A]).$$  \hfill (21)

For the evaluation of each model, we repeat our testing experiments $l = 900$ times for each of three models. We therefore define the average (absolute or relative) vector of eigenvalues – computed over the different estimates of the eigenvalues for the same model.

**Definition 10** Given a set of spectral differences $\left\{\Delta^{(k)}_\lambda\right\}_{k=1}^s$, computed over $l$ independent trials, the average absolute difference per eigenvalue is the $n$-dimensional vector given by,

$$\bar{\Delta}_\lambda = \frac{1}{l} \sum_{k=1}^l \Delta^{(k)}_\lambda.$$  \hfill (22)

**Definition 11** Given a set of spectral relative differences $\left\{\Delta^p_\lambda^{(k)}\right\}_{k=1}^s$, computed over $s$ independent trials, the average relative difference per eigenvalue is the $n$-dimensional vector given by,

$$\bar{\Delta}_\lambda^p = \frac{1}{l} \sum_{k=1}^l |\Delta^p_\lambda^{(k)}|.$$  \hfill (23)

### 6.1.1 The distance between the degree distributions.

The fine scale statistics, such as the degree distribution, provides a “window” on patterns of connectivity that happen at a fine local scale (the egonet). This small scale statistic is worthy of attention because large communities in real networks can be decomposed into smaller scale communities, which become more and more connected, as they become smaller (Leskovec et al, 2009). The degree distribution quantifies the finest scale “atomic” communities that cannot be further reduced.

Given a graph $G = (V, E)$ of size $n$, we use the histogram $f_n$ of degrees to characterize the degree distribution, defined as follows

$$f_n(k) = \frac{n_k}{n}$$  \hfill (24)

where $n_k$ is the number of vertices in $V$ with degree $k$. To compare two degree histograms, $f_n$ and $g_n$, we use the Kullback-Leibler divergence (Kullback and Leibler, 1951) given by

$$D_{KL}(f_n, g_n) = \sum_{k=1}^{n} f_n(k) \log \left( \frac{f_n(k)}{g_n(k)} \right).$$  \hfill (25)
The smaller the value of $D_{KL}(f_n, g_n)$ the closer the two distributions are to one another.

### 6.2 A pedestrian tour of the testing process.

To help provide some understanding into the testing process, we provide a tour of the testing process (for a specific model: SBM-Unet). Other models are evaluated in the same manner.

After having trained the convolutional neural network, we test the algorithm with a sample of adjacency matrices $A_1, \ldots, A_N$. We first compute the sample mean adjacency matrix $\bar{E}[A]$, which is the input to our algorithm. Our algorithm returns $\mu^*_N$, our estimate of the sample Fréchet mean. We then compute the eigenvalues $\lambda(\hat{\mu}_N)$ and $\lambda(\mu^*_N)$, and the vectors of errors in the eigenvalues, $\Delta(\hat{\mu}_N, \mu^*_N)$, and their relative versions $\Delta^p(\hat{\mu}_N, \mu^*_N)$.

Fig. 3-left displays (in red) the 28 eigenvalue errors, $\Delta(\hat{\mu}_N, \mu^*_N)$, while Fig. 3-right displays the relative errors $\Delta^p(\hat{\mu}_N, \mu^*_N)$. In addition, we also display (in blue) the error between sample mean spectrum, $\bar{E}[\lambda]$, and the spectrum of our estimate of the Fréchet mean, $\lambda(\mu^*_N)$.

The visual inspection of Fig. 3 suggests that the spectral differences, $\Delta(\hat{\mu}_N, \mu^*_N)$ (red curve) between the predicted adjacency matrix $\mu^*_N[A]$ and the true Fréchet mean $\hat{\mu}_N[A]$, is maximal for $\lambda_2$. Interestingly, the sample mean spectrum $\lambda(\bar{E}[A])$ remains very close to $\lambda(\mu^*_N[A])$ (except for the first eigenvalue).

Next, we calculate the degree distributions both for the predicted sample Fréchet mean graph, $\mu^*_N[G]$, as well as the true sample Fréchet mean graph, $\hat{\mu}_N[G]$ (see Fig. 4).

![Fig. 3](image_url) The vector of eigenvalues errors $\Delta(\hat{\mu}_N, \mu^*_N)$ (in red) and $\Delta(\mu^*_N[A], \bar{E}[\lambda])$ (in blue). Left: absolute error; right: relative error.
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We notice in Fig. 4 that while the distributions appear to be fairly different, SBM-Unet is able to accurately capture the peak corresponding to a degree of 13 in the true sample Fréchet mean graph, $\hat{\mu}_N[G]$. The KL divergence between the two distributions is approximately 3.8.

7 Results and Discussion

In general, we find that at least one of our models performs better than the naive $\tilde{\mu}_N$ both in terms of $\Delta_\lambda(\tilde{\mu}_N, \hat{\mu}_N)$ and $\Delta_\lambda^p(\hat{\mu}_N, \tilde{\mu}_N)$. This suggests that our models are able to better predict large scale structures of the sample Fréchet mean than the naive model. The spectral error between our prediction and the naive model is significantly smaller for the first eigenvalue, and remains lower up to the fifth or sixth eigenvalue.

When comparing the eigenvalues of the predicted Fréchet mean, $\lambda(\mu^*_N)$, and the sample mean vector of eigenvalues $\bar{E}[\lambda]$, we find that on average the eigenvalues from the Fréchet means computed with our models are closer to the sample mean eigenvalues than the eigenvalues predicted by the naive model $\lambda(\tilde{\mu}_N A)$.

Finally, with regard to the degree distributions we find it is often the case that our models produce degree distributions that are closer in terms of KL divergence to the true sample Fréchet mean graph, $\hat{\mu}_N[G]$ than to the naive $\tilde{\mu}_N[G]$.

7.1 Inhomogeneous Erdős-Rényi Testing Data

When the four models were evaluated using inhomogeneous Erdős-Rényi random graphs, IER-Unet and Gen-Unet resulted in the lowest spectral
approximation error (see Fig. 5). In contrast, both the IER-Unet and Gen-Unet had virtually identical $\Delta_{\lambda}(\hat{\mu}_N, \mu_N^*)$ and $\Delta_{\lambda}^p(\hat{\mu}_N, \mu_N^*)$, and performed worse than the naive model.

Fig. 5 provides a plot of the entries of the spectral differences $\Delta_{\lambda}(\hat{\mu}_N, \mu_N^*)$ and $\Delta_{\lambda}^p(\hat{\mu}_N, \mu_N^*)$. Tables 1 and 2 provide some basic statistics for both
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\[ \Delta \lambda(\hat{\mu}_N, \mu^*_N) \] and \[ \Delta \lambda^p(\hat{\mu}_N, \mu^*_N) \], including the maxima and minima of the entries, as well as the index of the corresponding minimum or maximum.

The comparison of the sample mean spectrum, \( \bar{\lambda}[\lambda] \) and the spectrum, \( \lambda(\mu^*_N) \) (see Fig. 6) reveals that all models perform relatively similarly in terms of \( \Delta \lambda(\lambda(\mu^*_N), \bar{\lambda}[\lambda]) \) and \( \Delta \lambda^p(\lambda(\mu^*_N), \bar{\lambda}[\lambda]) \). Overall, all our models achieve a smaller spectral error than the naive model. This results implies that our models, regardless of the training data, are able to capture the connectivity information that controls the eigenvalues of the adjacency matrix, irrespective of the training data. This result is not surprising, since Gen-Unet and IER-Unet were both presented with inhomogeneous Erdős-Rényi training data, and therefore we expected them to be able to predict the Erdős-Rényi graphs with high precision.

### Table 1 \( \Delta \lambda(\hat{\mu}_N, \mu^*_N) \) statistics for Erdős-Rényi generated testing data

| Model    | \( \max \Delta \lambda \) | \( \lambda^\max_{\Delta \lambda} \) | \( \min \Delta \lambda \) | \( \lambda^\min_{\Delta \lambda} \) |
|----------|----------------------------|----------------------------|-----------------------------|----------------------------|
| IER-Unet | 0.912596                   | 1                          | 0.060550                    | 28                         |
| SBM-Unet | 2.048245                   | 1                          | 0.066471                    | 28                         |
| PA-Unet  | 2.449364                   | 1                          | 0.069327                    | 28                         |
| Gen-Unet | 0.708872                   | 1                          | 0.058604                    | 28                         |
| Naive    | 1.840880                   | 1                          | 0.063173                    | 28                         |

### Table 2 \( \Delta \lambda^p(\hat{\mu}_N, \mu^*_N) \) statistics for Erdős-Rényi generated testing data, \( \max \Delta \lambda^p \) is over the first 10 eigenvalues only.

| Model    | \( \max \Delta \lambda^p \) | \( \lambda^\max_{\Delta \lambda^p} \) | \( \min \Delta \lambda^p \) | \( \lambda^\min_{\Delta \lambda^p} \) |
|----------|----------------------------|----------------------------|-----------------------------|----------------------------|
| IER-Unet | 0.080035                   | 1                          | 0.060586                    | 6                          |
| SBM-Unet | 0.212734                   | 1                          | 0.105618                    | 4                          |
| PA-Unet  | 0.244647                   | 1                          | 0.111006                    | 4                          |
| Gen-Unet | 0.070039                   | 10                         | 0.057397                    | 4                          |
| Naive    | 0.215085                   | 1                          | 0.078074                    | 6                          |

### Table 3 KL divergence for the inhomogeneous Erdős-Rényi testing data

| Model    | Mean     | Variance |
|----------|----------|----------|
| IER-Unet | 0.6066   | 0.0737   |
| SBM-Unet | 0.9588   | 0.2772   |
| PA-Unet  | 0.9899   | 0.0488   |
| Gen-Unet | 0.4133   | 0.04877  |
| Naive    | 0.4610   | 0.0675   |
When comparing the degree distributions of the true Fréchet mean graph, \( \widehat{\mu}_N[G] \), and that of the predicted sample Fréchet mean, \( \mu^*_N[G] \), we again confirm that both IER-Unet and Gen-Unet have lowest average KL divergence (see Table 3).

### 7.2 Stochastic Block Model Testing Data

When evaluated using stochastic block model data, all of our models perform better than the naive model in terms of \( \Delta_\lambda(\widehat{\mu}_N, \mu^*_N) \) and \( \Delta^p_\lambda(\widehat{\mu}_N, \mu^*_N) \). Somewhat surprisingly, PA-Unet, performs the best out of all our models followed closely by SBM-Unet (see Fig 7).

The evaluation of the spectral difference between the eigenvalues of the predicted Fréchet mean and the sample mean eigenvalues, \( \Delta_\lambda(\lambda(\mu^*_N), \widehat{E}[\lambda]) \) and \( \Delta^p_\lambda(\lambda(\mu^*_N), \widehat{E}[\lambda]) \), indicate that on average, up until the third eigenvalue, PA-Unet and SBM-Unet perform the best (see Fig. 8). However, after the third eigenvalue the naive model has the lowest values of \( \Delta_\lambda(\lambda(\mu^*_N), \widehat{E}[\lambda]) \) and \( \Delta^p_\lambda(\lambda(\mu^*_N), \widehat{E}[\lambda]) \), although the spectral difference does appear to converge towards zero as the eigenvalue increase for each model (see Fig. 8).

The change in model performance after the third eigenvalue suggests that our models are better predicting and representing the salient structural features of the sample, however they may not be picking up other spectral information as well as the naive model. Indeed, we know that the spectrum of the adjacency matrix of the SBM is composed of a bulk centered around zero,

![Fig. 7 Stochastic Block Model testing data: error between the eigenvalues of the true and predicted Fréchet mean for each model; absolute error \( \Delta_\lambda(\widehat{\mu}_N, \mu^*_N) \) for the first 25 eigenvalues (left); relative error for the first five eigenvalues, \( \Delta^p_\lambda(\widehat{\mu}_N, \mu^*_N) \) (right).](image-url)
Fig. 8 Stochastic Block Model testing data: spectral difference between the eigenvalues of the predicted Fréchet mean and the sample mean eigenvalues; absolute difference $\Delta_{\lambda}(\lambda(\mu^*_N), \bar{E}[\lambda])$ for the first 5 eigenvalues (left); relative difference for the first five eigenvalues, $\Delta^p_{\lambda}(\lambda(\mu^*_N), \bar{E}[\lambda])$ (right).

Table 4 KL divergence statistics for Stochastic Block Model generated testing data

| Model   | Mean   | Variance |
|---------|--------|----------|
| IER-Unet | 0.5034 | 0.0911   |
| SBM-Unet | 0.4366 | 0.0419   |
| PA-Unet  | 0.5996 | 0.0488   |
| Gen-Unet | 0.3684 | 0.0244   |
| Naive    | 0.4334 | 0.0476   |

and three positive eigenvalues – each associated with a corresponding community. Our models are therefore able to accurately predict the three dominant eigenvalues outside of the bulk, but miss the eigenvalues in the bulk.

When comparing the degree distribution of the true sample Fréchet mean graph, $\tilde{\mu}_N[G]$, to that of the predicted sample Fréchet mean graph, $\mu^*_N[G]$, we find that Gen-Unet achieves the lowest KL divergence (along with lower variance) (see Table 4).

7.3 Preferential Attachment Testing Data

Preferential attachment models have long been favored for their similarities to real world networks. However as we have discussed, less is known analytically about the eigenvalues of the preferential attachment model. We find that all of our models perform better than the naive model, $\tilde{\mu}_N$, in terms of $\Delta_{\lambda}(\tilde{\mu}_N, \mu^*_N)$ and $\Delta^p_{\lambda}(\tilde{\mu}_N, \mu^*_N)$. While the naive model produces an average absolute relative difference of approximately 10% for the first eigenvalue, the error jumps to 35%
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Fig. 9 Preferential attachment testing data: error between the eigenvalues of the true and predicted Fréchet mean for each model; absolute error $\Delta_\lambda (\hat{\mu}_N, \mu^*_N)$ for the first 25 eigenvalues (left); relative error for the first five eigenvalues, $\Delta^p_\lambda (\hat{\mu}_N, \mu^*_N)$ (right).

Fig. 10 Preferential attachment testing data: spectral difference between the eigenvalues of the predicted Fréchet mean and the sample mean eigenvalues; absolute difference $\Delta_\lambda (\lambda(\mu^*_N), \bar{E} [\lambda])$ for the first 5 eigenvalues (left); relative difference for the first five eigenvalues, $\Delta^p_\lambda (\lambda(\mu^*_N), \bar{E} [\lambda])$ (right).

for the fifth eigenvalue (see Fig. 9-right). In contrast, the error created by the PA-Unet model is less than 3.5% for the first eigenvalue, and is bounded by 10% for the fifth eigenvalue (see Fig 9-right).

Our experiments demonstrate that all our other models perform remarkably well compared to the naive model model. This results suggest that our algorithm can estimate the sample Fréchet mean for a wide variety of graph
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topology (not just IER, or SBM). These results are promising as preferential attachment models aim to capture the "scale-free" property present in many real world graph degree distributions.

The spectral difference between the eigenvalues of the predicted Fréchet mean and the sample mean eigenvalues are minimum (across the first five eigenvalues) for the model trained with the SBM data, SBM-Unet, (see Fig. 10). All of our models result in smaller differences than the naive model, $\tilde{\mu}_N$, until the third eigenvalue. This result is indeed very surprising considering that SBM-Unet was not trained on preferential attachment data so we would not expect it to perform as well as it does. The SBM-Unet is probably able to reproduce the large hubs that are present in the preferential attachment graphs, and which mimic the connectivity associated with the communities present in the SBM training data. These large hubs correspond to the dominant eigenvalues of the adjacency matrix.

Turning our attention to the comparisons between degree distributions, we find that all our models produce on average values of the KL divergence between the true and predicted sample Fréchet mean graphs that are lower than those of the naive model (see Fig. 5).

| Model    | Mean  | Variance |
|----------|-------|----------|
| IER-Unet | 0.4872| 0.0496   |
| SBM-Unet | 0.3109| 0.0250   |
| PA-Unet  | 0.3598| 0.0224   |
| Gen-Unet | 0.4208| 0.0262   |
| Naive    | 0.4970| 0.0378   |

8 Conclusion

We have described a fast method to compute the sample Fréchet mean graph using convolutional neural networks. The Fréchet mean graph has become a fundamental concept for graph-valued machine learning. Our approach relies on a combination of two key ideas: (i) stochastic block models with community of various sizes provide universal approximants to graphs, and (ii) the computation of the sample Fréchet mean of stochastic block models (sampled from the same probability measure) can be performed using simple averaging and nonlinear thresholding. We designed a convolutional network, which learns the combined optimal approximation of the graphs in a sample along with the averaging and nonlinear thresholding that yields the sample Fréchet mean. Our experiments on several ensembles of random graphs demonstrate that our method can reliably predict the sample Fréchet mean.

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