Graphon estimation via nearest neighbor algorithm and 2D fused lasso denoising

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Abstract

We propose a class of methods for graphon estimation based on exploiting connections with non-parametric regression. The idea is to construct an ordering of the nodes in the network, similar in spirit to Chan and Airoldi (2014). However, rather than only considering orderings based on the empirical degree as in Chan and Airoldi (2014), we use the nearest neighbor algorithm which is an approximating solution to the traveling salesman problem. This in turn can handle general distances \( \hat{d} \) between the nodes, something that allows us to incorporate rich information of the network. Once an ordering is constructed, we formulate a 2D grid graph denoising problem that we solve through fused lasso regularization. For particular choices of the metric \( \hat{d} \), we show that the corresponding two-step estimator can attain competitive rates when the true model is the stochastic block model, and when the underlying graphon is piecewise Hölder or it has bounded variation.

Keywords: total variation denoising, graph denoising, fused lasso, network estimation

1 Introduction

Suppose we are given measurements \( A_{i,j} \in \{0, 1\} \) with \( i,j \in \{1, \ldots, n\} \), and with

\[
\begin{align*}
A_{j,i} & = A_{i,j}, & \forall i,j \in \{1, \ldots, n\}, \\
A_{i,i} & = 0, & \forall i \in \{1, \ldots, n\}, \\
A_{i,j} & \sim \text{Bernoulli} \left( \theta_{i,j}^* \right), & \forall i < j, \ i,j \in \{1, \ldots, n\}, \\
\theta_{i,j}^* & = f_0(\xi_i, \xi_j), \\
\xi_i & \sim \text{i.i.d} \ U[0, 1], & i \in \{1, \ldots, n\},
\end{align*}
\]

(1)

where \( f_0 : [0, 1] \times [0, 1] \rightarrow [0, 1] \) is a function that might depend on \( n \). Moreover, the indices \( i \) and \( j \) denote the nodes of a network with \( n \) vertices, and \( A_{i,j} = 1 \) indicates that there is an edge between \( i \) and \( j \). The goal is to estimate \( \theta_{i,j}^* \), the probability that there is a link between \( i \) and \( j \), under structural assumptions of the function \( f_0 \).

The model described in (1) has attracted significant attention in the statistics and machine learning community. This is due to the increasing amount of data that can be represented as a binary graph model. For instance, emails between individuals, social networks connections, financial networks where an edge indicates a transaction between individuals, and many more.

The goal of this paper is to study a class of methods that can perform well in practice, yet they can enjoy attractive statistical properties under different classes of functions. We are particularly interested in settings where \( f_0 \) is piecewise Hölder, has bounded variation, or is an instance of the stochastic block model.
idea is based on the connection between nonparametric regression and graphon estimation, see Gao et al. (2015) for a discussion. Roughly speaking, we construct a 2D grid graph of size $n \times n$ by using information from the data $A$, and then we solve an optimization of problem of the form

$$\min_{\theta \in \mathbb{R}^{n \times n}} \frac{1}{2} \| A - \theta \|_F^2 + \lambda \| D\theta \|_1,$$

(2)

where $D : \mathbb{R}^{n \times n} \to \mathbb{R}^{2n(n-1)}$ is a linear operator, $\| \cdot \|_F$ is the Frobenius norm, and $\| \cdot \|_1$ is the usual $\ell_1$ norm, see the notation section below. The detailed construction of $D$ will be given later.

Essentially, we perform total variation denoising on the adjacency matrix $A$, treating its entries as nodes of carefully designed grid graphs. The first type of grid that we consider is constructed as follows. We consider $\{1, \ldots, n\}$ as cities with distances between them given by the metric from Zhang et al. (2015), thus the distance between $i$ and $j$ is

$$\hat{d}_I(i, j) = \frac{1}{n} \max_{k \neq i, j} \left| \sum_{l=1}^{n} (A_{i,l} - A_{j,l}) A_{k,l} \right|.$$

Using such metric, we run the nearest neighbor (NN) algorithm, which is an approximate solution to the traveling salesman problem, see for instance Rosenkrantz et al. (1977a). This gives a permutation $\hat{\tau}(1), \ldots, \hat{\tau}(n)$ of the nodes that can be used to embed the matrix $A$ in a 2D grid. With the embedding we can then solve a problem in the form of (2). We refer to the resulting procedure as NN-FL, given that it combines the NN algorithm with fused lasso regularization. Here, fused lasso refers to the estimator for denoising problems introduced by Tibshirani et al. (2005), whose predecessor is the total variation denoising estimator from Rudin et al. (1992). Equation (2) is actually a graph fused lasso denoising problem as studied from a theoretical perspective in Padilla et al. (2016) and Hutter and Rigollet (2016), and from an algorithmic point of view in Barbero and Sra (2014) and Tansey and Scott (2015). We exploit these algorithms in order to efficiently compute our estimator.

The second approach that we study considers an alternative to the distance form Zhang et al. (2015). Basically, we simply sort the degrees of the nodes just as in Chan and Airoldi (2014). However, once the ordering is obtained, we do not use the penalty in (3) as in Chan and Airoldi (2014) but rather we employ the fused lasso penalty. Hence we refer to the resulting procedure as SAS-FL, to emphasize that is a minor modification of the sort and smooth (SAS) method from Chan and Airoldi (2014). This small difference between SAS-FL and the method from Chan and Airoldi (2014) allows us to study the former on classes of bounded variation. We refer the reader to Sadhanala et al. (2016) for a discussion on some advantages of using the fused lasso on grids.

Finally, we will also discuss other possible choices of metrics such as those based on external data (independent of $A$), or the $\ell_1$ distance on the columns of $A$.

### 1.1 Summary of results

As stated above, our approach to graphon estimation is based on performing fused lasso/total variation denoising of the adjacency matrix with appropriate graphs. Loosely speaking, for the resulting estimators we show the following:

1. If the function $f_0(u, \cdot)$ is piecewise Hölder of exponent $\alpha \in (0, 1/2]$, then the NN-FL estimator attains the rate $n^{-\alpha/2}$ after disregarding logarithmic terms. In fact, our result actually holds for a class of functions larger than that of piecewise Hölder functions of exponent $\alpha$.

2. Let $g$ be the degree function $g(u) = \int f_0(u, v) \, dv$. If there exists a constant $L > 0$ such that $L |u - v| \leq |g(u) - g(v)|$ for all $u, v \in [0, 1]$, $g$ is piecewise–monotone, and $f_0$ has bounded variation, then the mean square error (MSE) of the SAS-FL attains rate $n^{-1/2}$ (if we ignore logarithmic terms).
3. We show that both NN-FL and SAS-FL attain the rate $K \log n/n$ when the true generative model is the stochastic block model with $K$ communities. This is similar to the performance of USVT which attains the rate $K/n$, as shown in Xu (2017). A minor difference is that the rate in Xu (2017) is on the expected mean squared error, whereas our upper bounds are concentration inequalities for the MSE.

4. In both simulated and real data examples, we provide evidence that the proposed methods outperform existing approaches for network denoising and link prediction.

1.2 Notation

For $n \in \mathbb{N}$ we denote the set $\{1, \ldots, n\}$ by $[n]$. Moreover, for $n \in \mathbb{N}$ we denote by $\mathcal{S}_n$, the set of permutations of $[n]$, thus bijections from $[n]$ to itself.

For a matrix $X \in \mathbb{R}^{s \times t}$, the $i$-th row of $X$ is denoted by $X_{i, \cdot}$, and the $i$-th column by $X_{\cdot, i}$. The Frobenius norm is denoted by

$$
\|X\|_F^2 = \sqrt{\sum_{i=1}^s \sum_{j=1}^t x_{i,j}^2}.
$$

For a set $I \subset [t]$ we denote by $X_{I, \cdot}$ the matrix obtained by removing from $X$ the columns whose indices correspond to elements in $[t] \setminus I$. We define $X_{I, I}$ in a similar way for $I \subset [s]$.

Throughout, we use the standard notation $\|x\|_p = \left( \sum_{i=1}^n |x_i|^p \right)^{1/p}$ for $x \in \mathbb{R}^n$, and $p \in \mathbb{N}$. We also use the notation $\|x\|_\infty = \max_{i \in [n]} |x_i|$.

For a Borel measurable set $A \subset \mathbb{R}^d$ we denote its Lebesgue measure in $\mathbb{R}^d$ by $\text{Vol}(A)$. And we denote by $1_A(x)$ the function that takes value 1 if $x \in A$ and 0 otherwise.

1.3 Previous work

Methods for network estimation have been extensively studied in the literature, and network denoising remains an active research area due to the challenge that it represents. One avenue of research has focused on assuming that the generative process is the stochastic block model. In such framework, the main difficulty is perhaps to estimate the communities to which the nodes belong. This perspective includes seminal works by Bickel and Chen (2009); Rohe et al. (2011) and Adamic and Glance (2005). More recent work includes that by Guédon and Vershynin (2016); Yan et al. (2018) among others.

In this paper we will not necessarily assume the stochastic block model but will also allow for more general models. Our work focuses on directly estimating the link probabilities to which we refer as graphon estimation. The statistical properties of graphon estimators have been of extensive interest. For instance, Airoldi et al. (2013) proposed to approximate Lipschitz graphons by block models, and consistency in Hölder classes was studied in Wolfe and Olhede (2013). Moreover, Gao et al. (2015) and Gao et al. (2016) characterized the minimax rates for graphon estimation under stochastic block model. The rate is $\log K/n$ where $K$, the number of communities, satisfies $K \leq \sqrt{n \log n}$. Recently, Xu (2017) and Klopp and Verzelen (2017) independently showed that the universal singular value thresholding (USVT) algorithm from Chatterjee et al. (2015) attains the rate $K/n$ when the true model is the stochastic block model. In fact, Xu (2017) shows the rate $K/(n \rho)$ where $\rho$ is a sparsity parameter that satisfies $n \rho = \Omega(\log n)$. The authors in Xu (2017) also studied USVT when the function $f_0$ (in Model 1) belongs to a Sobolev space.

Moreover, Zhang et al. (2015) studied graphon estimation under more general structures than the stochastic block model. The method from Zhang et al. (2015) proceeds in a two–step fashion. First, a network with nodes $\{1, \ldots, n\}$ is constructed using the adjacency matrix $A$. Then, neighborhood smoothing is applied to the different neighborhoods. The resulting estimator is proven to be consistent in the case in which $f_0$
is piecewise Lipschitz. The respective rate is \((\log n/n)^{1/2}\) versus the minimax rate \(\log n/n\). A different method was studied in Song et al. (2016) that is also based on neighborhood smoothing.

An alternative approach to graphon estimation considering degree sorting was studied in Chan and Airoldi (2014) under the assumption that \(f_0(x, y)dy\) is increasing. The idea behind this method is to construct an ordering of the nodes based on the empirical degree \(d_i = \sum_{j=1}^{n} A_{i,j}\). Once the ordering is obtained, Chan and Airoldi (2014) proposes the sort and smooth (SAS) estimator

\[
\hat{\theta}_{sas} = \arg \min_{\theta} \sum_{i=1}^{m} \sum_{j=1}^{m} \sqrt{\left( \frac{\partial \theta}{\partial x} \right)^2_{i,j} + \left( \frac{\partial \theta}{\partial y} \right)^2_{i,j}} \text{ subject to } \|\theta - H\|_2 \leq \epsilon, \tag{3}
\]

where \(\epsilon > 0\) is a tuning parameter, and \(H\) is a smooth version of \(A\), \(\frac{\partial \theta}{\partial x} \left( \frac{\partial \theta}{\partial y} \right)\) is a discrete derivative in the direction of the \(x\) \((y)\) axis.

Finally, we emphasize that while several graphon estimation methods exist, many properties of estimators are unknown. For instance, the estimator from Zhang et al. (2015) is consistent when the true graphon is piecewise Lipschitz but it is unknown whether such estimator can be nearly minimax when the true model is the stochastic block model. Also, USVT can perform well under the stochastic block model assumption or some smooth condition on \(f_0\), but performance guarantees are unknown when \(f_0\) is piecewise Hölder or it is a general bounded variation function.

## 2 General approach

In this section we propose a general class of estimators filling in the details of our discussion in Section 1. We begin by reviewing some background on the traveling salesman problem. This is then related to the graphon estimation problem given rise to our family of estimators.

### 2.1 Nearest neighborhoods construction

Our approach to construct a grid graph is motivated by the traveling salesman problem. We describe this in generality next. Let \(C = \{c_1, \ldots, c_s\}\) be a set of cities with a distance metric \(d_C : C \times C \rightarrow \mathbb{R}\) specifying how far any pair of cities are from each other. A tour of cities is a sequence \(c_{P(1)}, \ldots, c_{P(s)}\) where \(P\) is a permutation of the set \(\{1, \ldots, s\}\). Thus, a tour is just an arrangement of cities such that each city appears exactly once.

The traveling salesmen problem (see Bellmore and Nemhauser (1968) for a survey) is a well known problem that seeks for the tour with the minimum cost, measuring the cost in terms of the metric \(d_C\), see below. The optimal tour or circuit is found by solving

\[
P^* \in \arg \min_{P \in S_s} C(P), \tag{4}
\]

where the cost of a tour \(P\) is defined as

\[
C(P) = \sum_{i=1}^{s-1} d_C(c_{P(i)}, c_{P(i+1)}) + d_C(c_{P(s)}, c_{P(1)}).
\]

Unfortunately, it is known that (4) is NP-hard, see for instance Rosenkrantz et al. (1977a). Despite this challenge, there exist different approximation algorithms for solving (4). For instance, Rosenkrantz et al. (1977a) studied approximation algorithms which run in polynomial time. From such methods, we will
mainly use the nearest neighbor algorithm (NN) which starts from a random city, and then proceeds iteratively by choosing the closest city to the current city. Specifically, at first the algorithm visits \( \hat{\tau}(1) \) for some \( \hat{\tau}(1) \in C \), perhaps chosen randomly. Next, the NN algorithm visits \( \hat{\tau}(2) \), where

\[
\hat{d}(\hat{\tau}(1), \hat{\tau}(2)) \leq d(\hat{\tau}(1), c), \quad \forall c \in C \setminus \{\hat{\tau}(1)\}.
\]

Then, the NN algorithm continues sequentially visiting \( \hat{\tau}(j) \) at iteration \( j \) where

\[
\hat{d}(\hat{\tau}(j - 1), \hat{\tau}(j)) \leq \hat{d}(\hat{\tau}(j - 1), c), \quad \forall c \in C \setminus \{\hat{\tau}(1), \ldots, \hat{\tau}(j - 1)\}.
\]

Although, the nearest neighbor method is straightforward, it enjoys some attractive performance guarantees. In particular, denoting the permutation associated with NN by \( \hat{P} \), Theorem 1 in Rosenkrantz et al. (1977a) shows that

\[
C(\hat{P}) \leq \left(1 + \frac{\log_2 s}{2}\right) C(P^*),
\]

provided that \( \hat{d} \) satisfies the triangle inequality.

Moreover, by its mere definition, one can see that the computational complexity of running the NN algorithm is \( O(ws^2) \), where \( w \) is the computational cost of evaluating \( d_C \).

### 2.2 Class of estimators

As anticipated, our approach is based on running 2D grid fused lasso denoising on the data \( A \) with a carefully constructed graph. Let us now state more precisely on how to arrive to our estimator \( \hat{\theta} \in \mathbb{R}^{n \times n} \) for \( \theta^* \).

In order to avoid correlation between the constructed ordering and the signal to denoise, for \( m \in [n] \) we use the data \( A_{\cdot, [m]} \) to construct metric \( \hat{d} : ([n] \setminus [m]) \times ([n] \setminus [m]) \to \mathbb{R} \). Once the metric is constructed, we can think of the elements of \( ([n] \setminus [m]) \) as a set of cities, and for any two cities \( i, j \in [n] \), the distance \( \hat{d}(i, j) \) tells us how far the cities are. The discussion on the choices of the metric \( \hat{d} \) will be given later.

**Choice of \( m \):** Throughout we assume that \( m \) is chosen to satisfy \( m \asymp n \), thus there exists positive constants \( c_1 \) and \( c_2 \) such that \( c_1 m \leq n \leq c_2 m \). For instance, we could take \( m = \lfloor n/2 \rfloor \).

A natural way to arrange the cities (nodes), in the graphon estimation problem, would be to place as adjacent cities that are close to each other in the sense of the metric \( \hat{d} \). This would make sense if the graphon has some underlying structure, for instance if the ground truth is the stochastic block model. We would also require that the distance \( \hat{d}(i, j) \) is a reasonable approximation to a metric \( d^*(\xi_i, \xi_j) \), such that \( f_0(\xi_i, \cdot) \) and \( f_0(\xi_j, \cdot) \) are “similar” if \( d^*(\xi_i, \xi_j) \) is small. We will be precise in stating our assumptions but for now we proceed to construct the proposed approach.

Motivated by the discussion above, we use the NN algorithm (as discussed in Section 2.1) on the cities \([n] \setminus [m]\) with distance \( \hat{d} \). We let \( \hat{\tau} \) be the corresponding function \( \hat{\tau} : [n - m] \to ([n] \setminus [m]) \), such that the NN algorithm first visits city \( \hat{\tau}(1) \), next city \( \hat{\tau}(2) \), and so on.

Using the ordering \( \hat{\tau} \), we construct a signal \( y \in \mathbb{R}^{(n - m) \times (n - m)} \) satisfying \( y_{i,j} = A_{\hat{\tau}(i), \hat{\tau}(j)} \) for all \( i, j \in [n - m] \). We also construct the 2D grid graph \( G = (V, E) \) with set of nodes

\[
V = \{(i, j) : i, j \in [n - m]\},
\]

and set of edges

\[
E = \{(e^-, e^+) \in [n - m]^2 \times [n - m]^2 : \|e^+ - e^-\|_1 = 1\}.
\]

We also use \( \nabla_G \) to denote an oriented incidence operator of \( G \). Thus, \( \nabla_G : \mathbb{R}^{(n - m) \times (n - m)} \to \mathbb{R}^{|E|} \) where for \( e = (e^+, e^-) \in E \) we have

\[
(\nabla_G \theta)_e = \theta_{e^+} - \theta_{e^-}.
\]
Using the graph $G$, we proceed to construct our estimator by solving a graph fused lasso problem. Thus, we first find $\hat{\beta} \in \mathbb{R}^{(n-m)\times(n-m)}$ as the solution to

$$
\minimize_{\beta \in \mathbb{R}^{(n-m)\times(n-m)}} \frac{1}{2}\|y - \beta\|_F^2 + \lambda \|
abla G\beta\|_1,
$$

for a tuning parameter $\lambda > 0$. We then set $\hat{\theta}_{\hat{i}(i),\hat{j}(j)} = \hat{\beta}_{ij}$ for all $i, j \in [n-m]$.

The procedure above allows us to estimate $\theta_{i,j}^*$ for all $i, j \in [m]$. In a similar way we can also construct estimates of $\theta_{i,j}^*$ for all $i, j \in [m]$. The idea is to have an ordering of the nodes in $[m]$ by using the NN algorithm with a metric that only involves data from $A_{i,[n]\setminus[m]}$, and then we solve a 2D fused lasso problem.

As for the estimates of $\theta_{i,j}^*$ for all $i \in [n]\setminus[m]$ and $j \in [m]$, we proceed in a similar way but using two different orderings. The first ordering $\hat{\tau}_1$ is obtained by running the NN algorithm on the set of cities $[m]$ with a metric depending on the data $A_{m,m}$. For the second ordering we use the NN algorithm with the set of cities $([n]\setminus[m])$ and metric depending the data $A_{([n]\setminus[m]),([n]\setminus[m])}$.

Finally, we emphasize that we do the portioning of the data in order to avoid correlation between the ordering and the signal to denoise. This is done to keep the analysis mathematically correct. However, in practice, one can obtain a single ordering and then run a fused lasso problem as in (2). We have noticed that such a approach works well in practice.

**Computational cost.** As stated in the previous subsection, the computational cost associated with the NN algorithm is $O(sn^2)$, where $s$ is the cost of computing the distance between any two nodes. Note that this can be reduced if there are multiple processors available. In such case, the distance from a node to the remaining nodes could be computed by partitioning the nodes and performing computations in parallel.

As for the fused lasso computation, this can be done using the efficient algorithm from Barbero and Sra (2014), or the ADMM solver from Tansey and Scott (2015) which is amenable to parallel computing.

### 2.3 Choices of metric $\hat{d}$

Clearly, the class of methods described above can be used with any metric $\hat{d}$ on the set of nodes on the graphon estimation. The purpose of this section is to highlight different choices of $\hat{d}$, some of which have appeared in the literature in the context of other estimators.

For simplicity, we will focus on constructing $\hat{d}$ for the case of estimating $\theta_{i,j}^*$ for all $i, j \in [n]\setminus[m]$. The remaining cases described in Section 2.2 can be constructed in a similar way.

#### 2.3.1 Inner product based distance

Our first natural approach for constructing $\hat{d}$ is to consider the metric proposed in Zhang et al. (2015). Specifically, we set

$$
\hat{d}_I(i, i') = \max_{k \in [m]} \frac{1}{n} | \langle A_{i,[m]}, A_{k,[m]} \rangle - \langle A_{i',[m]}, A_{k,[m]} \rangle |, \quad \forall i, i' \in [n]\setminus[m].
$$

We call NN-FL the estimator from Section 2.2 when the distance $\hat{d}$ is taken as $\hat{d}_I$ in (7).

Importantly, our modification of the distance defined in Zhang et al. (2015) does satisfy the triangle inequality, which is important for the NN algorithm to satisfy (5).
2.3.2 Sorting

Another choice for the distance $\hat{d}$ is

$$\hat{d}(i, i') = \frac{1}{m} \left| \sum_{j \in [m]} A_{i,j} - \frac{1}{m} \sum_{j \in [m]} A_{i',j} \right|, \quad \forall i, i' \in [n] \setminus [m].$$

Thus, for any two nodes, the distance is the absolute value of the difference between the degrees (normalized by $m$) based on the data $A_{i,[m]}$. Since such degrees are numbers and the metric is the Euclidean distance, the optimal tour (traveling salesman problem solution) is the ordering obtained by sorting the degrees. This is the ordering constructed in the method from Chan and Airoldi (2014). The difference is that we use the fused lasso penalty for denoising without preliminary smoothing of the data, whereas Chan and Airoldi (2014) uses the penalty in (3) with an smoothed version of $A$.

Throughout, whenever we use the distance (8) we will refer to the estimator from Section 2.2 as sort and smooth fused lasso graphon estimation (SAS-FL). In this experiments section we will see that, as expected, the empirical performance of SAS-FL is similar to SAS from Chan and Airoldi (2014), although the former seems to perform sightly better in the examples we considered.

2.3.3 $\ell_1$ distance and other choices

Clearly, a different metric can be obtained by simply taking the $\ell_1$ norm of the difference between rows or columns of the incidence matrix $A$. Thus, we can define

$$d_{\ell_1}(i, i') = \|A_{i,[m]} - A_{i',[m]}\|_1, \quad \forall i, i' \in [n] \setminus [m].$$

We will refer to the respective procedure using this metric as $\ell_1$-FL. We will not study convergence properties of this method, although we will see that it is a reasonable method in practice.

Finally, we notice that the metric $\hat{d}$ could be constructed using side information about the nodes. For instance, using covariates, or repeated measurements of the network if available.

3 Analysis of the NN-FL estimator

The purpose of this section is to study convergence proprieties of the NN-FL estimator. We organize our results into two subsections to highlight different classes of functions.

3.1 Extensions of piecewise Hölder classes

We start by analyzing the performance of the NN-FL estimator for classes of graphons that extent the notion of piecewise Hölder functions. We notice that a particular instance of this was studied in Zhang et al. (2015).

To formalize, if $\alpha \in (0, 1)$, we say that $f_0$ is piecewise Hölder of exponent $\alpha$ if the following holds:

There exists a partition of intervals $A_1, \ldots, A_r$ of $[0, 1]$, such that if $u, v \in A_l$ for some $l \in [r]$, then

$$\sup_{t \in [0,1]} |f_0(u, t) - f_0(v, t)| \leq L_1 |u - v|^{\alpha},$$

and

$$\sup_{t \in [0,1]} |f_0(t, u) - f_0(t, v)| \leq L_1 |u - v|^{\alpha},$$

for a positive constant $L_1$ independent of $u$ and $v$. 


This class of functions appeared in the analysis of the fused lasso estimator in the context of 2D non-parametric regression, see Hutter and Rigollet (2016). There, the authors showed that the fused lasso attains the rate $n^{-\alpha/(1+\alpha)}$.

Next, we state two assumptions which hold if (9) is satisfied along with Model 1. Thus, we relax the piecewise Hölder condition.

**Assumption 1.** There exists a positive constant $c_1$ such that with probability approaching one
\[
\min_{k \in [m]} \int_0^1 |f_0(x_k, t) - f_0(x_i, t)| dt \leq c_1 \left( \frac{\log n}{n} \right)^\alpha, \quad \forall i \in [n] \setminus [m].
\]
and
\[
\min_{k \in [m]} \int_0^1 |f_0(t, x_k) - f_0(t, x_i)| dt \leq c_1 \left( \frac{\log n}{n} \right)^\alpha, \quad \forall i \in [n] \setminus [m].
\]
for $\alpha \in (0, 1/2]$.

Note that we constrain $\alpha \in (0, 1/2]$, and the case $\alpha \in [1/2, 1]$ will not be studied. Instead, we will analyze the stochastic block model in the next subsection.

To see why Assumption 1 holds when condition (9) is met with $\alpha \in (0, 1/2]$, we appeal to the work in Von Luxburg et al. (2010). There, the authors showed that, with probability approaching one, the following holds: For each $\xi_i$, the set of its $K$-th nearest neighbors (with Euclidean distance) among the points $\{x_j\}_{j \in [n] \setminus \{i\}}$ are all within distance $c \log n/n$ for an appropriate choice of $K$, and for some constant $c > 0$.

We now state our second assumption. This involves the quantity that the penalty $\|\nabla_G \cdot \|_1$ in (6) emulates.

**Assumption 2.** There exists an unknown (random) permutation $\tau^* \in \mathcal{S}_{n-m-1}$ such that
\[
\sum_{i=1}^{n-m-1} \int_0^1 |f_0(\xi_{\tau^*(i)}, t) - f_0(\xi_{\tau^*(i+1)}, t)| dt = O_P(n^{1-\alpha} \log^\alpha n),
\]
and
\[
\sum_{i=1}^{n-m-1} \int_0^1 |f_0(t, \xi_{\tau^*(i)}) - f_0(t, \xi_{\tau^*(i+1)})| dt = O_P(n^{1-\alpha} \log^\alpha n),
\]
where $\alpha \in (0, 1/2]$.

If (9) and (10) hold then Assumption 2 will be satisfied. To see this, simply take $\tau^*$ as the ordering of the elements of $\{\xi_i\}_{i \in ([n]\setminus m]}$ as
\[
\xi_{\tau^*(1)} < \xi_{\tau^*(2)} < \ldots < \xi_{\tau^*(n-m)}.
\]
Once again, we exploit the characterization on nearest neighbor graphs from Von Luxburg et al. (2010).

With these conditions, we are now ready to present our next result.

**Theorem 1.** Let us suppose that Assumptions 1-2 hold, and let $\hat{\tau}$ be constructed as in Section 2.2 by setting $d := \hat{\alpha}_t$ (see Equation 7). Then for an appropriate choice of $\lambda$, the corresponding estimator in (6) from Section 2.2 satisfies
\[
\frac{1}{n^2} \sum_{i,j \in [n-m], i < j} \left( \hat{\theta}_{\hat{\tau}(i), \hat{\tau}(j)} - \theta^*_{\hat{\tau}(i), \hat{\tau}(j)} \right)^2 = O_P \left( \frac{\log^2 + \alpha}{n^2 \frac{\alpha}{2}} \right).
\]

Thus, in the class implied by Assumptions 1–2, the NN-FL estimator attains the rate $n^{-\alpha/2}$ after ignoring logarithmic terms. To the best of our knowledge, other estimators have not been studied on this class of functions. The most related work comes from Zhang et al. (2015) who studied piecewise Lipschitz for which their estimator attains the rate $n^{-1/2}$.
3.2 Stochastic block model

Given the wide popularity of the stochastic block model, we proceed to analyze the convergence rate of the estimator SAS-FL under such model. We start by stating the underlying assumption in the stochastic block model.

**Assumption 3.** The signal $\theta^*$ satisfies

$$\theta^*_{i,j} = \rho f_0(\xi_i, \xi_j),$$

such that

$$f_0(x, y) = \sum_{k,k'=1}^{K_n} Q_{k,k'} 1_{\{x \in A_k\}} 1_{\{y \in A_{k'}\}},$$

where $A_1 = [a_0, a_1)$ with $a_0 = 0$, and $A_k = [a_{k-1}, a_k]$ for $k \in \{2, \ldots, K_n\}$ with $a_{K_n} = 1$. Note that we have allowed the number of pieces to depend on the sample size. We write $\hat{\theta}_{i,j} = \theta^*_{i,j}/\rho$, $\hat{Q}_{k,k'} = Q_{k,k'}/\rho$ and the goal is to estimate $\hat{\theta}$.

We recall that the parameter $K_n$ in Assumption 3 refers to the number of communities. The corresponding model can be thought as consisting of a set of disjoint communities, where each node belongs to a community, and the probability of a link between two nodes only depends on the communities to which the nodes belong.

Note that we have allowed for an overall sparsity parameter $\rho$, although the focus of this paper are not sparse networks.

We now show that the NN-FL estimator attains a competitive performance in estimation when the stochastic block model holds. We will focus on the case $\rho = 1$, although we expect that our estimator will be competitive even in sparse settings. A result for more general values of $\rho$ will be given in the next section for SAS-FL.

To proceed, we first show that the metric $\hat{d}_I$, defined in Equation (7), concentrates around a certain metric involving the link probabilities.

**Lemma 2.** With $\hat{d}_I$ defined as in (7), there exist positive constants $C_1$ and $C_2$ such that

$$|\hat{d}_I(i, i') - d_I(i, i')| \leq \sqrt{2C_1 \left( \frac{\log n}{n} \right)^{1/4}}, \quad \forall i, i' \in [n]\setminus[m],$$

with probability at least $1 - n^{-C_2}$ where

$$d_I(i, i') = \max_{k \in \text{[m]}} \sqrt{\frac{1}{m} |\langle \theta^*_{k,[m]}, \theta^*_{k',[m]} \rangle - \langle \theta^*_{k,[m]}, \theta^*_{k',[m]} \rangle|}, \quad \forall i, i' \in [n]\setminus[m].$$

Hence, that the metric $\hat{d}_I$ approximates the distance $d_I$ which compares nodes using the link probabilities. The key is that if two nodes belong to the same community, i.e if the latent variables $\xi_i$ and $\xi_j$ belong to the same interval $A_l$, with the notation from Assumption 3, then $d_I(i, j) = 0$. In such case the distance $\hat{d}_I(i, j)$ is driven by noise. In contrast, if $i$ and $j$ are not in the same community ($\xi_i \in A_l$, $\xi_j \in A_{l'}$, with $l \neq l'$), then $d_I(i, j) \neq 0$. And hence the distance $\hat{d}_I(i, j)$ would behave like $d_I(i, j)$ if the noise is dominated by the latter. We state this condition below and then prove that leads to the rate $K \log n/n$.

**Assumption 4.** The probability of the event $\{C_l \cap [m] \neq \emptyset \ \forall l \in K_n\}$ approaches to 1 as $n$ goes to infinity. Moreover,

$$\frac{1}{\sqrt{2}} \sqrt{\sum_{s=1}^{K_n} \frac{n_l}{n} (Q_{l,s} - Q_{l',s})^2} > 2 \sqrt{2C_1 \left( \frac{\log n}{n} \right)^{1/4}}$$

with probability approaching 1, where $C_1$ is the constant from Corollary 2.
Note that condition above can be stated in terms of the volume of the sets $A_l$ as the quantities $n_l/n$ concentrate around such numbers by concentration measure. However, Assumption 4 is more general and hence it might be preferred.

In addition, the requirement that the event $\{C_l \cap [m] \neq \emptyset \ \forall \ l \in K_n\}$ happens with probability approaching one follows immediately by Proposition 27 in Von Luxburg et al. (2010). This holds provided that

$$n \min_{l \in [K_n]} \text{Vol}(A_l) \to \infty,$$

for the sets $A_l$ from Assumption 3.

We are now ready to state our next result. The result is comparable to recent developments for other estimators like USVT, see Xu (2017). However, we emphasize that NN-FL can perform well in this simple yet important case, as well as more general frameworks such as the one described in Section 3.1.

**Theorem 3.** Let us suppose that Assumptions 3 and 4 hold with $\rho = 1$. Let $\hat{\tau}$ be constructed as in Section 2.2 by setting $d := \hat{d}_I$. Then for an appropriate choice of $\lambda$, the corresponding estimator in (6) from Section 2.2 satisfies

$$\frac{1}{n^2} \sum_{i,j \in [n-m], i < j} \left( \hat{\theta}(i) \cdot \hat{\tau}(j) - \theta^*_\tau(i) \cdot \hat{\tau}(j) \right)^2 = O_P \left( \frac{K_n \log n}{n} \right).$$

Thus, the previous theorem shows that NN-FL attains the rate $K \log n/n$ when the ground truth is the stochastic block model. The purposes of this theorem is not to market NN-FL as the ideal method for stochastic block model, since for instance, USVT has, in expectation, an upper bound of the order $K/n$.

Rather, from this and the previous subsections we see that NN-FL can be competitive under a broad range of function classes.

### 4 Analysis of the SAS-FL estimator

#### 4.1 BV functions

The first class of graphons considered includes the assumption of bounded variation. This condition has appeared in the statistics literature due to its flexibility in that it encompasses a very large class of functions that includes reasonable subclasses such as piecewise Lipschitz. In one dimensional non-parametric regression, Mammen and van de Geer (1997) studied locally adaptive estimators that attain minimax rates when the true regression function has bounded variation. More recently, Tibshirani and Taylor (2011); Tibshirani (2014) studied discretized version of the estimators from Mammen and van de Geer (1997). The framework from Section 2.2 consists of a particular instance of generalized lasso estimation studied in Tibshirani and Taylor (2011).

In one dimension, bounded variation is well defined as follows. A function $f : [0, 1] \to \mathbb{R}$ has bounded variation if there exists a constant $C$ such that for any set of points $0 \leq a_1 \leq \ldots \leq a_r \leq 1$, $r \in \mathbb{N}$, it holds that

$$\sum_{l=1}^{r-1} |f(a_l) - f(a_{l+1})| < C.$$  \hspace{1cm} (12)

When passing to higher dimensions (in particular dimension two), the definition of bounded variation is not unique. See for instance Clarkson and Adams (1933), an early work discussing multiple definitions of bounded variation. Although these days there is a widespread convention in the definition of bounded variation in the field of mathematics, the statistics community continues relying on early definitions. For instance, perhaps implicitly Sadhanala et al. (2016) defines the canonical class of bounded variation by
taking (12) and assuming it holds through each horizontal and vertical chain graph of a 2D grid graph. We now do something similar for the case of graphons.

**Assumption 5.** We assume the data is generated as in the model implied by (1). Moreover, we assume that the functions

\[ g_1(u) = \int_0^1 f_0(u, v) dv, \quad g_2(u) = \int_0^1 f_0(v, u) dv \]

satisfy:

1. There exists some positive constant \( L_1 \) such that
   \[ L_1 |x - y| \leq |g_l(x) - g_l(y)|, \quad \forall x, y \in [0, 1], \forall l \in \{1, 2\}. \tag{13} \]

2. **Piecewise-Monotonic:** For \( l \in \{1, 2\} \) there exists a partition \( 0 < b_1^l < \ldots < b_r^l < 1 \) such that \( g_l \) is monotone in each of the intervals \((0, b_1^l), (b_1^l, b_2^l), \ldots, (b_r^l, 1)\).

3. The function \( f_0 \) has **bounded variation** in the following sense. There exists a positive constant \( C > 0 \) such that if \( 0 \leq a_0 \leq a_1 \leq \ldots \leq a_s \leq 1 \) with \( s \in \mathbb{N} \), then
   \[ \sum_{l=1}^{s-1} |f_0(a_l, t) - f_0(a_{l+1}, t)| < C, \]

   and
   \[ \sum_{l=1}^{s-1} |f_0(t, a_l) - f_0(t, a_{l+1})| < C, \]

for all \( t \in [0, 1] \).

Importantly, we allow for a flexibility of the graphon by only requiring that has bounded variation. The most restrictive assumption is perhaps that \( g \) is piecewise monotonic. As for the condition expressed by (13), we note that this requirement appeared in the analysis in Chan and Airoldi (2014).

**Theorem 4.** Suppose that Assumption 5 holds, then we have that

\[ \frac{1}{n^2} \sum_{i,j \in [n-m], i<j} \left( \hat{\theta}_{\hat{\tau}(i), \hat{\tau}(j)} - \tilde{\theta}_{\hat{\tau}(i), \hat{\tau}(j)} \right)^2 = O_p \left( \frac{\log^2 n}{\sqrt{n}} \right). \]

Thus, on the class of functions from Assumption 5, the SAS-FL estimator attains the rate \( n^{-1/2} \), which matches the theoretical result from Zhang et al. (2015) but for the class of piecewise Lipschitz functions.

Interestingly, we are the first to study graphon estimation with the bounded variation assumption.

### 4.2 Stochastic block model

We now consider the performance of the SAS-FL estimator when the stochastic block model stated in Assumption 3 holds. Unlike the analysis of NN-FL, our next result includes cases where the sparsity parameter converges to zero. The corresponding theorem is presented next.
Theorem 5. Let us set $q_l = a_l - a_{l-1}$ and $\Delta_l = \sum_{s=1}^{K_n} q_{ls} \tilde{Q}_{ls}$ for $l \in [K_n]$. Let us assume that there exists a sequence $\delta_n \downarrow 0$ such that

\[
\left(\frac{\delta_n^2 \min_{l \in [K_n]} \Delta_l}{\log n}\right) \frac{\rho n}{\log n} \to \infty, \quad \frac{\delta_n^2 n \min_{l \in [K_n]} q_l}{\log n} \to \infty,
\]

(14)

and

\[
\frac{\min_{l \neq l', l, l' \in [K_n]} |\Delta_l - \Delta_{l'}|}{\delta_n} \to \infty,
\]

(15)

Then under Assumption 3, we have that

\[
\frac{1}{n^2} \sum_{i,j \in [n-m], i < j} \left( \frac{1}{\rho} \hat{\theta}_{\hat{\tau}(i), \hat{\tau}(j)} - \tilde{\theta}_{\hat{\tau}(i), \hat{\tau}(j)} \right)^2 = O_p \left( \frac{K_n \log n}{n \rho} \right).
\]

Let us now clarify the quantities involved in the previous theorem. The first of these is the length of the $l$-th interval denoted as $q_l$, which is the probability that a given node belongs to community $l$ (the respective latent variable is in $A_l$). The quantity $\Delta_l$ is the normalized (divided by $\rho$) expected degree of the nodes in community $l$. Equation (14) then puts a constraint on the parameter $\rho$ although it includes scenarios where such parameter can approach zero. As for (15), this requires that different communities have different expected degrees.

Finally, we see that SAS-FL attains the same rate $K_n/(\rho n)$ (ignoring logarithm terms) as the expected mean squared error associated with USVT. Note that the result for SAS-FL is more restrictive than that for USVT as the latter can handle smaller values of $\rho$. However, our result is a concentration inequality whereas the rate for USVT is in expectation. In addition, the SAS-FL can also adapt to general functions as described in Section 4.1.

5 Experiments

The purpose of this section is to shed some lights as to the empirical performance of the class of estimators proposed in this paper. Evaluations of performance are presented next on both simulated and real networks.

5.1 Network denoising

We begin by considering examples of simulated data that are intended to test the validity of our general class of methods on qualitatively different scenarios. The specifications of $\hat{d}$ that we consider are those described in Section 2.3.

As benchmarks we consider the following approaches. The neighborhood smoothing method (NS) from Zhang et al. (2015), universal singular value thresholding (USVT) algorithm from Chatterjee et al. (2015), and the sort and smooth (SAS) method from Chan and Airoldi (2014).

In all comparisons, the MSE is used as a measure of performance. Four different scenarios are constructed. In the first scenario the ground truth is the stochastic block model with 12 communities. In our second example, $f_0$ is taken as piecewise smooth, where locally the function behaves like linear combinations of the $\sqrt{\cdot}$ function applied to each coordinate. We also consider a piecewise constant model (not a stochastic block). In the latter, the degree function behaves locally as a constant making estimation difficult for both SAS and SAS-FL. Our final example consists $f_0$ being a polynomial of two variables. For a visualization of the examples, we refer the reader to Figures 1-4.
Figure 1: The top left in the first row shows a realization of the matrix of probabilities \( P \) for Example 1, here \( n = 500 \). Then from left to right the panels in the first row correspond to the methods SAS, USVT, and NS. In the second row the leftmost plot corresponds to a realization of the incidence matrix (A) drawn with the parameters in \( P \) from the first row. Then from left to right the remaining plots are associated to SAS-FL, NN-FL, and \( \ell_1 \)-FL.

Figure 2: The top left in the first row shows a realization of the matrix of probabilities \( P \) for Example 2, here \( n = 500 \). Then from left to right the panels in the first row correspond to the methods SAS, USVT, and NS. In the second row the leftmost plot corresponds to a realization of the incidence matrix (A) drawn with the parameters in \( P \) from the first row. Then from left to right the remaining plots are associated to SAS-FL, NN-FL, and \( \ell_1 \)-FL.
Figure 3: The top left in the first row shows a realization of the matrix of probabilities $P$ for Example 3, here $n = 500$. Then from left to right the panels in the first row correspond to the methods SAS, USVT, and NS. In the second row the leftmost plot corresponds to a realization of the incidence matrix (A) drawn with the parameters in $P$ from the first row. Then from left to right the remaining plots are associated to SAS-FL, NN-FL, and $\ell_1$-FL.

Figure 4: The top left in the first row shows a realization of the matrix of probabilities $P$ for Example 4, here $n = 500$. Then from left to right the panels in the first row correspond to the methods SAS, USVT, and NS. In the second row the leftmost plot corresponds to a realization of the incidence matrix (A) drawn with the parameters in $P$ from the first row. Then from left to right the remaining plots are associated to SAS-FL, NN-FL, and $\ell_1$-FL.
Table 1: Simulation results for Examples 1, 2, 3 and 4, see Figures 1–4 in that order. Comparisons between the true and estimated probability matrices for different methods given samples from each example. The acronyms here are given the text. The Mean squared error (MSE) is multiplied by a constant.

(a) Mean squared error, times 1000, averaging over 50 Monte Carlo simulations, for different methods given samples from Example 1.

| n   | NN-FL | L1-FL | SAS-FL | SAS  | USVT | NS  |
|-----|-------|-------|--------|------|------|-----|
| 500 | 2.8   | 4.9   | 13.5   | 15.2 | 5.1  | 3.9 |
| 1000| 1.5   | 2.7   | 10.5   | 13.1 | 2.1  | 2.5 |
| 2000| 1.2   | 1.6   | 9.2    | 12.3 | 1.6  | 1.9 |

(b) Mean squared error, times 1000, averaging over 50 Monte Carlo simulations, for different methods given samples from Example 2.

| n   | NN-FL | L1-FL | SAS-FL | SAS  | USVT | NS  |
|-----|-------|-------|--------|------|------|-----|
| 500 | 1.7   | 4.2   | 0.9    | 1.0  | 1.9  | 2.9 |
| 1000| 1.0   | 2.4   | 0.47   | 0.53 | 0.82 | 1.7 |
| 2000| 0.88  | 1.7   | 0.33   | 0.35 | 0.55 | 1.3 |

(c) Mean squared error, times 1000, averaging over 50 Monte Carlo simulations, for different methods given samples from Example 3.

| n   | NN-FL | L1-FL | SAS-FL | SAS  | USVT | NS  |
|-----|-------|-------|--------|------|------|-----|
| 500 | 8.2   | 9.9   | 56.5   | 60.7 | 9.4  | 8.7 |
| 1000| 5.7   | 6.3   | 47.9   | 59.7 | 6.4  | 6.4 |
| 2000| 5.1   | 5.0   | 44.6   | 59.4 | 5.3  | 5.3 |

(d) Mean squared error, times 1000, averaging over 50 Monte Carlo simulations, for different methods given samples from Example 4.

| n   | NN-FL | L1-FL | SAS-FL | SAS  | USVT | NS  |
|-----|-------|-------|--------|------|------|-----|
| 500 | 2.0   | 4.3   | 1.3    | 1.4  | 1.8  | 3.6 |
| 1000| 1.3   | 2.5   | 0.67   | 0.71 | 0.88 | 2.2 |
| 2000| 1.1   | 1.9   | 0.48   | 0.50 | 0.59 | 1.7 |

For the methods based on fused lasso denoising, namely SAS-FL, NN-FL, and ℓ₁-FL we choose the tuning parameter λ by cross-validation. This is done by selecting the best value of λ out of 30 candidates, by erasing 20% of the data points and replacing them by zeros, and then performing predictions based on the remaining data.

The results for each scenario are given in Table 1. These are obtained by averaging over 50 Monte Carlo simulations, and for values of \( n \in \{500, 1000, 1500\} \). From Table 1, we see that in most cases the best method is either NN-FL or SAS-FL. Even for the stochastic block model example, the method NN-FL seems to have the best performance.

Moreover, in Example 3, we see that SAS and SAS-FL suffer greatly due to the nearly constant behavior of the degree function \( (g_1, g_2) \) in Assumption 5). In contrast, NN-FL and ℓ₁-FL are not affected by the degree issue and offer strong performance.

Figures 1-4 allow us to visualize the comparisons of different methods in the examples considered. In Figure 1, we can see that NN-FL gives a more detailed recovery of the blocks compared to all the other methods. As for Figure 2, we see that with \( n = 500 \), all the competing methods are comparable, although, based on MSE, SAS-FL is the best approach. In Figure 3, we clearly see the effect of the degree on the performance of SAS and SAS-FL.
Table 2: Average AUC-ROC for the competing methods under Examples 1 and 2.

| Example | NN-FL | ℓ₁-FL | SAS-FL | SAS | USVT | NS |
|---------|-------|--------|--------|-----|------|----|
| 1       | 0.84  | 0.83   | 0.76   | 0.84| 0.60 | 0.69|
| 2       | 0.92  | 0.93   | 0.80   | 0.82| 0.39 | 0.92|

5.2 Link prediction

We now validate the methods studied in this paper in the task of link prediction. To that end, we consider two different datasets. For our first example we use the Protein230 dataset from Butland et al. (2005). This consists 230 proteins and their interactions encoded in 595 edges. In our second example, we use the Yeast protein interaction network from Butland et al. (2005). This is a larger network consisting of 2361 nodes and 6646 edges.

Using the data described above, we evaluate the prediction performance of different methods as follows. In each case, we remove some observations of the matrix $A \in \mathbb{R}^{n \times n}$, thus rather than observing $A$, we assume that the data is $\tilde{A}$ where

$$\tilde{A}_{i,j} = \rho_{i,j} A_{i,j}, \quad \rho_{i,j} \sim \text{i.i.d.} \text{Bernoulli}(0.8), \quad \forall i, j \in [n].$$

For each data example we generate 50 trials of $\tilde{A}$, and for each instance of $\tilde{A}$ we fit different estimators. For each estimator we compute the area under the curve (AUC) of the receiver operating characteristic (ROC). We then report the average AUC-ROC and refer to it simply as AUC-ROC.

With the setting described above, Table 2 reports the average AUC-ROC associated to the competing methods in each of the considered examples. We can see that for both examples, NN-FL and ℓ₁-FL are the most competitive estimators. As a sanity check, we also computed the area under the precision recall curve, and found that in both cases the best approach was NN-FL.

6 Conclusion

We have studied a novel class of graphon estimators based on a two–step approach that combines the nearest neighbor algorithm with the graph fused lasso. Overall the estimators seem to perform reasonably in both simulated and real data.

Statistical guarantees have been provided, although some questions remain open. For instance, we have not studied the statistical performance when the graphon is piecewise Hölder with exponent in the interval $[1/2, 1]$.

We also leave for future work to understand the convergence properties ℓ₁-FL which also seems like a reasonable approach, at least in the examples considered here.

A Proofs

We assume that $f_0(x, y) = f_0(y, x)$ for all $x, y \in [0, 1]$. This is not important in the proofs but it makes the arguments rely in simpler notation.

A.1 Important lemmas

First we recall Theorem 2 from Hoeffding (1963).
Let $\epsilon$ also assume that the coordinates of random permutation independent of $\epsilon$ where $D$ addition, we assume that $s$ assume that for each $j$ for some constant $C > 0$, then $N$ Lemma 8. $c$ where $E$ independence assumption, and the third inequality is met by Lemma 2.2 from Boucheron et al. (2013).

Proof. Simply note that

$$\mathbb{E}\left(\epsilon \sum_{i=1}^{d} s_i \epsilon_{\hat{P}(i)}\right) = \mathbb{E}\left(\mathbb{E}\left(\epsilon \sum_{i=1}^{d} s_i \epsilon_{\hat{P}(i)} \mid \hat{P}\right)\right) = \mathbb{E}\left(\prod_{i=1}^{d} \mathbb{E}\left(e^{s_i \epsilon_{\hat{P}(i)}} \mid \hat{P}\right)\right) \leq \mathbb{E}\left(\prod_{i=1}^{d} e^{s_i^{2}/2}\right) = e^{\|s\|^{2}/2},$$

where the first equality follows from the tower property of expectations, the second equality holds by the independence assumption, and the third inequality is met by Lemma 2.2 from Boucheron et al. (2013).

Lemma 7. Let $\epsilon \in \mathbb{R}^d$ a random vector and let $\hat{P} \in S_d$ be random permutation such that $\epsilon \| \hat{P}$. If the coordinates of $\epsilon$ are independent with mean zero and belong to $[-1, 1]$, then

$$\mathbb{E}\left(\epsilon \sum_{i=1}^{d} s_i \epsilon_{\hat{P}(i)}\right) \leq e^{\|s\|^{2}/2}, \quad \forall s \in \mathbb{R}^d.$$

Proof. Letting $\tilde{\epsilon} \epsilon_{\hat{P}(i)}$, we proceed as in the basic inequality argument from the proof of Theorem 3 in Wang et al. (2016).

Theorem 6. (Hoeffding) Let $Z_1, \ldots, Z_n$ be centered independent random variables satisfying $\alpha \leq Z_i \leq \beta$ for all $i = 1, \ldots, n$. Then, for all $\delta > 0$, we have, with probability at least $1 - \delta$, that

$$\left|\frac{1}{n} \sum_{i=1}^{n} Z_i\right| \leq \sqrt{\frac{c \log (2/\delta)}{2n}},$$

where $c = n^{-1} \sum_{i=1}^{n} (a_i - b_i)^2$.

Lemma 7. Let $\epsilon \in \mathbb{R}^d$ a random vector and let $\hat{P} \in S_d$ be random permutation such that $\epsilon \| \hat{P}$. If the coordinates of $\epsilon$ are independent with mean zero and belong to $[-1, 1]$, then

$$\mathbb{E}\left(\epsilon \sum_{i=1}^{d} s_i \epsilon_{\hat{P}(i)}\right) \leq e^{\|s\|^{2}/2}, \quad \forall s \in \mathbb{R}^d.$$

Proof. Simply note that

$$\mathbb{E}\left(\epsilon \sum_{i=1}^{d} s_i \epsilon_{\hat{P}(i)}\right) = \mathbb{E}\left(\mathbb{E}\left(\epsilon \sum_{i=1}^{d} s_i \epsilon_{\hat{P}(i)} \mid \hat{P}\right)\right) = \mathbb{E}\left(\prod_{i=1}^{d} \mathbb{E}\left(e^{s_i \epsilon_{\hat{P}(i)}} \mid \hat{P}\right)\right) \leq \mathbb{E}\left(\prod_{i=1}^{d} e^{s_i^{2}/2}\right) = e^{\|s\|^{2}/2},$$

where the first equality follows from the tower property of expectations, the second equality holds by the independence assumption, and the third inequality is met by Lemma 2.2 from Boucheron et al. (2013).

Lemma 8. (Minor modification to Corollary 5 from Hutter and Rigollet (2016) Consider the model

$$y_i = \mu_i^* + \epsilon_i, \quad i = 1, \ldots, m = N_1 \times N_2,$$

with $N_i/N = z_i$ for some $z_i \in \mathbb{N}$, $l = 1, 2$. Here $N$ is a quantity that can grow to infinity. Moreover, we assume that for each $j \in [m]$ we have that $\epsilon_j = \epsilon_i$ for some $i \in [\tilde{m}]$, where $\epsilon \in \mathbb{R}^{\tilde{m}}$ with $\tilde{m} \gg m$. In addition, we assume that $s_i = |\{j \in [m] \mid \epsilon_j = \epsilon_i\}| \leq \kappa$ for all $i \in [\tilde{m}]$, for some positive constant $\kappa$. We also assume that the coordinates of $\epsilon = (\epsilon_1, \ldots, \epsilon_{\tilde{m}})$ are independent and satisfy $\mathbb{E}(\epsilon_i) = 0, \epsilon_i \in [-1, 1]$. Let

$$\hat{\mu} = \arg\min_{\mu \in \mathbb{R}^m} \frac{1}{2} \sum_{i=1}^{m} (y_{\hat{P}(i)} - \mu_i)^2 + \lambda m \|D\mu\|_1,$$

where $D$ is the incidence matrix of $N_1 \times N_2$ grid graph, $\lambda > 0$ is a tuning parameter, and $\hat{P} \in S_{\tilde{m}}$ is a random permutation independent of $\epsilon$. Then there exists a constant $c > 0$ such that for any $\delta > 0$, if $\lambda$ is chosen as

$$\lambda = \frac{c \log N \sqrt{\log (\kappa m / \delta)}}{m},$$

then

$$\mathbb{P}\left(\frac{1}{m} \|\hat{\mu} - \mu^*\|_2^2 \geq C \frac{\log m \sqrt{2 \log (\kappa m / \delta)} \|D\mu^*\|_1 + \log^2 m \log (\epsilon / \delta)}{m}\right) < \frac{2 z_1 z_2}{\delta},$$

for some constant $C > 0$.

Proof. We proceed as in the basic inequality argument from the proof of Theorem 3 in Wang et al. (2016). Letting $\tilde{\epsilon} = (\epsilon_{\hat{P}(1)}, \ldots, \epsilon_{\hat{P}(m)})$, we obtain

$$\frac{1}{2} \|\hat{\mu} - \mu^*\|_2^2 \leq \tilde{\epsilon}^T (\hat{\mu} - \mu^*) + m \lambda \|D\mu^*\|_1 - \|D\hat{\mu}\|_1.$$  (16)
Note that there exists two disjoint subsets $A_1, A_2, \ldots, A_{z_1 \cdot z_2}$ of $\{1, \ldots, m\}$ such that in the graph with incidence matrix $D$, the elements of $A_1$ lie on sub-grid graph of dimensions $N \times N$, the elements of $A_2$ lie on a different sub-grid of dimensions $N \times N$ and so on. Throughout, for a vector $\mu \in \mathbb{R}^{N_1 \times N_2}$, we write $\mu^j = (\mu^j_{i_1}, \ldots, \mu^j_{i_{N_2}})$ where $i_1^j < \ldots < i_{N_2}^j$, with $A_j = \{i_1^j, \ldots, i_{N_2}^j\}$ for $j = 1, 2, \ldots, z_1 \cdot z_2$.

Moreover, we denote by $D^j$ the incidence matrix of grid graph with dimensions $N \times N$.

Using the notation above, and writing $\Pi$ as the projection onto the span of $1 \in \mathbb{R}^{N_2}$, we obtain that there exists permutation matrices $P_1, \ldots, P_{z_1 \cdot z_2} \in \mathbb{R}^{N_2 \times N_2}$ such that

$$
\tilde{\varepsilon}^T (\hat{\mu} - \mu^*) = \sum_{j=1}^{z_1 \cdot z_2} (\tilde{\varepsilon}^j)^T (\hat{\mu}^j - (\mu^*)^j)
= \sum_{j=1}^{z_1 \cdot z_2} \left[ (\Pi \tilde{\varepsilon}^j)^T (\hat{\mu}^j - (\mu^*)^j) + ((I - \Pi) \tilde{\varepsilon}^j)^T (\hat{\mu}^j - (\mu^*)^j) \right]
\leq \sum_{j=1}^{z_1 \cdot z_2} \| (\Pi \tilde{\varepsilon}^j) \|_2 \| \hat{\mu}^j - (\mu^*)^j \|_2 + \max_{1 \leq j \leq z_1 \cdot z_2} \| ((D^j)^T P_j \tilde{\varepsilon}^j) \|_\infty \| ||D \mu^*||_1 + ||D \hat{\mu}||_1 \]
$$

where we have proceeded as in the proof of Theorem 2 from Hutter and Rigollet (2016), using Hölder’s inequality. Now, for $x \in \mathbb{R}^{N_2}$ we have that

$$
x^T \tilde{\varepsilon}^j = \sum_{l=1}^{N_2} x_l \tilde{\varepsilon}^j_{i_l} = \sum_{l=1}^{N_2} x_l \varepsilon_{P(i_l)} = \sum_{s=1}^{\tilde{m}} \varepsilon_s \left( \sum_{l : P(i_l) = \varepsilon_s} x_l \right) =: \tilde{x}^T \varepsilon
$$

where $\tilde{x} \in \mathbb{R}^{\tilde{m}}$ and satisfies

$$
\| \tilde{x} \|_2 = \sqrt{\sum_{s=1}^{\tilde{m}} \left( \sum_{l : P(i_l) = \varepsilon_s} x_l \right)^2} \leq \sqrt{\kappa} \| x \|_2.
$$

Therefore, combining the above observation with Lemma 7, and Corollary 2.6 from Boucheron et al. (2013), and (17) it follows that

$$
\tilde{\varepsilon}^T (\hat{\mu} - \mu^*) \leq 2 \kappa^{1/2} \sqrt{2 \log(e/\delta)} \| \hat{\mu} - \mu^* \|_2 + \rho \kappa^{1/2} \sqrt{2 \log(e N^2/\delta)} \| ||D \mu^*||_1 + ||D \hat{\mu}||_1
$$

with probability at least $1 - 2 z_1 z_2 / \delta$, where as in Proposition 4 from Hutter and Rigollet (2016), there exists a constant $c_1 > 0$ such that $\rho \leq c_1 \sqrt{\log m}$.

Therefore, combining (16) with (18) and using the inequality $a x - x^2 / 4 \leq a^2$ for all $a$ and $x$, we arrive to the conclusion.

\[\square\]

### A.2 Proof of Theorem 4

Let $\sigma$ and $\tau$ be bijections such that

$$
\xi_{\sigma(1)} < \ldots < \xi_{\sigma(n-m)},
\quad
\eta(\xi_{\tau(1)}) < \ldots < \eta(\xi_{\tau(n-m)}),
$$

where $\sigma(i), \tau(i) \in [n] \setminus [m]$.

We write $\ell(i) := l$ if $\xi_i \in A_l$.  

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Lemma 9. Let us assume that $n \leq c_2 m$. Then, the event

$$\Omega = \left\{ \xi : \max_{i \in [n]/\{m\}} \left| g(\xi_i) - \frac{1}{m} \sum_{j \in [m]} A_{i,j} \right| \leq 2 c_2 \left( \frac{\log n}{n} \right)^{\frac{1}{2}} \right\},$$

happens with probability at least $1 - \frac{4}{n}$.

Proof. First we observe that by Theorem 6 and union bound

$$\mathbb{P} \left( \max_{i \in [n]/\{m\}} \left| \frac{1}{m} \sum_{j \in [m]} A_{i,j} - \sum_{j \in [m]} \theta_{i,j}^* \right| > \sqrt{c_2} \left( \frac{\log n}{n} \right)^{\frac{1}{2}} \right) \leq \frac{2}{n}. \quad (19)$$

Next we define the set

$$\tilde{\Omega} = \left\{ \xi : \max_{i \in [n]/\{m\}} \left| g(\xi_i) - \frac{1}{m} \sum_{j \in [m]} \theta_{i,j}^* \right| \leq \sqrt{c_2} \left( \frac{\log n}{n} \right)^{\frac{1}{2}} \right\}, \quad (20)$$

and by Theorem 6 (and using conditional probability) we have that $\mathbb{P} \left( \tilde{\Omega} \right) \geq 1 - 2/n$. Now,

$$\mathbb{P} \left( \max_{i \in [n]/\{m\}} \left| \frac{1}{m} \sum_{j \in [m]} A_{i,j} - g(\xi_i) \right| \leq 2 c_2 \left( \frac{\log n}{n} \right)^{\frac{1}{2}} \right) \geq \int_{\tilde{\Omega}} \mathbb{P} \left( \max_{i \in [n]/\{m\}} \left| \frac{1}{m} \sum_{j \in [m]} A_{i,j} - g(\xi_i) \right| \leq 2 c_2 \left( \frac{\log n}{n} \right)^{\frac{1}{2}} \right) d\xi$$

$$\geq \int_{\tilde{\Omega}} \mathbb{P} \left( \max_{i \in [n]/\{m\}} \left| \frac{1}{m} \sum_{j \in [m]} A_{i,j} - \sum_{j \in [m]} \theta_{i,j}^* \right| \leq c_2 \left( \frac{\log n}{n} \right)^{\frac{1}{2}} \right) d\xi \geq [1 - \frac{2}{n}] \int_{\tilde{\Omega}} d\xi \geq 1 - \frac{4}{n}. \quad (21)$$

\hfill \square

Lemma 10. Let us assume that $c_1 m \leq n \leq c_2 m$. Then the event $\tilde{\Omega}$ given as

$$\max_{i \in [n]/\{m\}} \left| \xi_{\sigma(i)} - \frac{i}{n - m} \right| \leq 2 c_2 \left( \frac{\log n}{n} \right)^{\frac{1}{2}},$$

happens with probability at least $1 - 2 \exp(-8 c_3 \log n / L_1^2)$ where $c_3 = c_2 (c_1 - 1)/c_1$.

Proof. This follows immediately from Dvoretzky–Kiefer–Wolfowitz inequality. \hfill \square

Lemma 11. Let $\Omega'$ be the event that

$$\forall i, j \in [n - m], |i - j| > \frac{12}{L_1} \sqrt{c_2 n \log n} \quad \text{implies} \quad |\xi_{\sigma(i)} - \xi_{\sigma(j)}| > \frac{8}{L_1} \left( \frac{c_2 \log n}{n} \right)^{\frac{1}{2}}.$$

Then $\mathbb{P} \left( \Omega' \right) \geq 1 - 2 \exp(-8 c_3 / L_1^2 \log n)$ with $c_3$ as in Lemma 10.
Proof. Let us assume that the event $\tilde{\Omega}$ from Lemma 10 holds. Let $i, j \in [n - m]$ such that $|\xi_{\sigma(i)} - \xi_{\sigma(j)}| < 8/L_1 \sqrt{c_2 \log n/n}$. Then

$$\left| \frac{i}{n - m} - \frac{j}{n - m} \right| \leq \left| \frac{i}{n - m} - \xi_{\sigma(i)} \right| + \left| \xi_{\sigma(i)} - \xi_{\sigma(j)} \right| + \left| \frac{j}{n - m} - \xi_{\sigma(j)} \right| < \frac{12}{L_1} \left( \frac{c_2 \log n}{n} \right)^{\frac{1}{2}},$$

and the claim follows from Lemma 10.

\[ \boxed{\text{Lemma 12.} \quad \text{The event} \quad \Omega_2 = \left\{ \max_{i \in [n]\setminus[m]} |\hat{\tau}^{-1}(i) - \tau^{-1}(i)| \leq \frac{24}{L_1} (c_2 n \log n)^{\frac{1}{2}} \right\} \}

happens with probability at least $1 - 4/n - 2 \exp(-8 c_3/L_1^2 \log n)$ with $c_3$ as in Lemma 10.

Proof. Let us assume that the events $\Omega$ and $\Omega'$ from Lemma 9 and Lemma 11 hold. Let also $i, i' \in [n - m]$ be such that $|i - i'| > 12(c_2 n \log n)^{1/2}/L_1$. Then,

$$8 \left( \frac{c_2 \log n}{n} \right)^{\frac{1}{2}} \leq L_1 \left| \xi_{\sigma(i)} - \xi_{\sigma(i')} \right| \leq \left| g(\xi_{\sigma(i)}) - g(\xi_{\sigma(i)}) \right|.$$

Therefore, for large enough $n$, if $|i - i'| > 12(c_2 n \log n)^{1/2}/L_1$ then

$$\sum_{j \in [m]} A_{\sigma(i),j} < \sum_{j \in [m]} A_{\sigma(i'),j} \quad \text{iff} \quad g(\xi_{\sigma(i)}) < g(\xi_{\sigma(i')}). \quad (22)$$

Next let us fix $i \in [n - m]$ and define

$$\Lambda_1 = \left\{ i' \in [n - m] : \sum_{j \in [m]} A_{\sigma(i),j} < \sum_{j \in [m]} A_{\sigma(i'),j} \right\}, \quad \Lambda_2 = \left\{ i' \in [n - m] : g(\xi_{\sigma(i)}) < g(\xi_{\sigma(i')}) \right\}$$

then if (22) holds then

$$|\hat{\tau}^{-1}(\sigma(i)) - \tau^{-1}(\sigma(i))| = ||\Lambda_1| - |\Lambda_2|| \leq \max\{|\Lambda_1 \setminus \Lambda_2|, |\Lambda_2 \setminus \Lambda_1|\} \leq 24(c_2 n \log n)^{1/2}/L_1.$$

\[ \boxed{\text{Theorem 13.} \quad \text{Let us suppose that Assumptions 5 hold. Let } \hat{\tau} \text{ be constructed as in Section 2.2 by setting } d := d_1. \text{ Then,} \}

$$\frac{1}{n^2} \sum_{i=1}^{n-m-1} \sum_{j=m+1}^{n} |\theta_{\hat{\tau}(i),j}^* - \theta_{\hat{\tau}(i+1),j}^*| = O_P \left( \sqrt{\frac{\log n}{n}} \right).$$

Proof. Let $\delta = 24(c_2 \log n)^{1/2}/(L_1 n^{1/2})$, $S' = \{b_1, \ldots, b_r\}$ and $\Lambda = \{ i : \xi_{\tau(i)} \notin B_\delta(S') \}$, where $B_\delta(S') = \{ x : |x - x'| < \delta, \text{ for some } x' \in S' \}$. We also write

$$T_i = \{ j \in [n]\setminus[m] : |\xi_j - \xi_{\tau(i)}| \leq \delta \}.$$

Then by Proposition 27 from Von Luxburg et al. (2010) we have that

$$\mathbb{P} \left( \min_{i \in [n-m]} T_i \geq (n - m) \delta \right) \geq 1 - (n - m) \exp \left( -\frac{n \delta}{6} \right),$$

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Moreover, for $i \in \Lambda$ and $i' = \tau^{-1}(\hat{\tau}(i))$ then
\[
|\xi_{\tau(i)} - \xi_{\hat{\tau}(i)}| = |\xi_{\tau(i)} - \xi_{\tau(i')}| + \frac{\sigma^{-1}(\tau(i))}{n-m} - \frac{\sigma^{-1}(\tau(i'))}{n-m} + |\xi_{\tau(i')} - \frac{s}{n-m}|
\leq \frac{4c_2}{L_1} \left( \frac{\log n}{n} \right)^{\frac{1}{2}} + \left| \frac{i}{n-m} - \frac{v'}{n-m} \right|
\leq \frac{28c_2}{L_1} \left( \frac{\log n}{n} \right)^{\frac{1}{2}},
\]
where in the second inequality we have used the fact that $\xi_{\tau(i)}$ and $\xi_{\tau(i')}$ belong to the same connected component of $[0,1] \setminus B_{\delta}(S')$, and the function $g$ is strictly piecewise monotonic.

The argument above implies that
\[
\max_{i \in \Lambda} \left| \frac{\xi_{\hat{\tau}(i)} - \sigma^{-1}(\tau(i))}{n} \right| \leq \frac{30}{L_1} \left( \frac{c_2 \log n}{n} \right)^{\frac{1}{2}}.
\]

We now let $\delta_2 = 150 (\log n)^{1/2} / (L_1 n^{1/2})$. We also let $s = \lfloor \delta_2 n \rfloor$, and clearly $s \asymp \sqrt{n \log n}$. Moreover, for $i \in \{0,1,\ldots,s-1\}$ we define $l_i = \lceil (1 - i/n) / (s/n) \rceil$ and
\[
B_i^0 = \left[ 0, \frac{i}{n} \right), \quad B_i^1 = \left[ \frac{i}{n}, \frac{i+s}{n} \right), \quad \ldots, \quad B_i^s = \left[ \frac{i+s(l_i-1)}{n}, \frac{i+sl_i}{n} \right), \quad B_i^{s+1} = \left[ \frac{i+sl_i}{n}, 1 \right].
\]

Then if $y_k^i, z_k^i \in B_i^k$ with $y_k^i < z_k^i$ and $k \in \{1,\ldots,l_i\}$, then by Assumption 5 we have that for any $j \in [n] \setminus [m]$
\[
\sum_{k=1}^{l_i} \left| f_0 \left( \frac{i+(k-1)s}{n}, \xi_j \right) - f_0 \left( y_k^i, \xi_j \right) \right| + \left| f_0 \left( y_k^i, \xi_j \right) - f_0 \left( z_k^i, \xi_j \right) \right| + \left| f_0 \left( z_k^i, \xi_j \right) - f_0 \left( \frac{i+ks}{n}, \xi_j \right) \right| \leq C.
\]

On the other hand, with probability approaching one,
\[
\left| \frac{\xi_{\hat{\tau}(i')}}{n} - \frac{\sigma^{-1}(\tau(i'))}{n} \right| \leq \frac{\delta}{4} \leq \frac{s}{4n}, \quad \left| \frac{\xi_{\hat{\tau}(i'+1)}}{n} - \frac{\sigma^{-1}(\tau(i'+1))}{n} \right| \leq \frac{\delta}{4} \leq \frac{s}{4n}, \quad \forall i' \in \Lambda.
\]

Next let $I = \{i' \in [n-m] : \xi_{\hat{\tau}(i')}, \xi_{\hat{\tau}(i'+1)} \in \left( \frac{1}{n} + \frac{s}{2n}, 1 - \frac{2s}{n} \right) \}$. Let us assume that (24) holds and let $i' \in I$. Then we set $i'' = \lfloor \sigma^{-1}(\tau(i')) - \frac{s}{4} \rfloor$ and observe that
\[
\xi_{\hat{\tau}(i')}, \xi_{\hat{\tau}(i'+1)} \in \left( \frac{i''}{n}, \frac{i''}{n} + \frac{s}{n} \right) = B_{\hat{\tau}(i')},
\]
where $\lfloor \sigma^{-1}(\tau(i')) - \frac{s}{4} \rfloor = r_{i'} + k_{i'} s$ with $r_{i'} \in \{0,1,\ldots,s-1\}$ and $k_{i'} \in [l_{r_{i'}}]$. Therefore using (23),
with probability approaching one we have that
\[
\sum_{j \in [n] \setminus [m]} \sum_{i=1}^{n-m-1} |f_0(\xi_{\hat{\tau}(i)}, \xi_j) - f_0(\xi_{\hat{\tau}(i+1)}, \xi_j)| \\
\leq 2n \|f_0\|_\infty (|[n] \setminus I| + |[n] \setminus \Lambda|) + \sum_{j \in [n] \setminus [m]} \sup_{s-1 \leq \ell_k < \ell_k \in B_k, i \in \{0, \ldots, s-1\}, k \in [l]} \sum_{i=0}^{l_i} \sum_{k=1}^{l} \left[ |f_0(y_k^i, \xi_j) - f_0(z_k^i, \xi_j)| \right] \\
\leq 2n \|f_0\|_\infty (|[n] \setminus I| + |[n] \setminus \Lambda|) + n s C,
\]
and by a binomial concentration inequality we have that
\[
|[n] \setminus I| + |[n] \setminus \Lambda| = O_p \left( \sqrt{n \log n} \right).
\]

\[\blacksquare\]

**Proof of Theorem 4:** This follows from the previous theorem combined with Lemma 8.

### A.3 Proof of Theorem 5

This follows from the following lemma combined with Lemma 8.

**Lemma 14.** Under the assumptions of Theorem 5 with probability approaching 1 the following holds. There exist \( i_1 < i_2 < i_{m-1} \) such that

\[
i, i' < i_1, \quad \xi_{\hat{\tau}(i)} \in A_l, \quad \xi_{\hat{\tau}(i')} \in A_{l'} \text{ implies } l = l',
\]

\[
j \leq i, i' < j + 1, \quad j \in [m-1] \{m-1\}, \quad \xi_{\hat{\tau}(i)} \in A_l, \quad \xi_{\hat{\tau}(i')} \in A_{l'}, \text{ implies } l = l',
\]

\[
i, i' \geq i_{m-1}, \quad \xi_{\hat{\tau}(i)} \in A_l, \quad \xi_{\hat{\tau}(i')} \in A_{l'} \text{ implies } l = l',
\]

**Proof.** We let \( N_i = \sum_{j \in [m]} A_{l,j} \) for \( i \in [n] \), and \( n_i = \{j \in [m] : \xi_j \in A_l\} \) for \( l \in [K_n] \). Then \( N_i = \{n_l\}_{i=1}^{K_n}, \theta^* \sim \text{Bin}(m, \frac{1}{m} \sum_{j \in [m]} \theta_j^*, \xi_j) \), and \( n_i \sim \text{Bin}(m, q_i) \) with \( q_i = a_i - a_{i-1} \).

On the other hand, there exist positive constants \( c_1 \) and \( c_2 \) such that \( c_1 n \leq m \leq c_2 n \). Therefore, by Proposition 27 in Von Luxburg et al. (2010) we have that for any \( \delta \in (0, 1) \)

\[
P( c_1 (1 - \delta) n q_i \leq n_i \leq c_2 (1 + \delta) n q_i ) \geq 1 - 2 \exp \left( -\frac{1}{3} \delta^2 c_1 n q_i \right).
\]

Next, let \( i \) such that \( \xi_i \in A_l \), and \( I_{l'} = [c_1 (1 - \delta) n q_i, c_2 (1 + \delta) n q_i] \) for all \( l' \in [K_n] \). Then

\[
P \left( (1 - \delta)^2 n \rho \left[ \sum_{l'=1}^{K_n} c_{l' q_i} \tilde{Q}_{l', l' \rho} \right] \leq N_i \leq (1 + \delta)^2 n \rho \left[ \sum_{l'=1}^{K_n} c_{l' q_i} \tilde{Q}_{l', l' \rho} \right] \right)
\]
\[
\geq \sum_{n_i^0 \in I_i, I_i \in [K_n]} P \left( (1 - \delta) \rho \left[ \sum_{l'=1}^{K_n} n_i^0 \tilde{Q}_{l', l' \rho} \right] \leq N_i \leq (1 + \delta) \rho \left[ \sum_{l'=1}^{K_n} n_i^0 \tilde{Q}_{l', l' \rho} \right] | n_i^0 = n_i, \forall l' \in [K_n] \right) \\
\cdot P (n_i = n_i^0, \forall l' \in [K_n])
\]
\[
\geq \sum_{n_i^0 \in I_i, I_i \in [K_n]} P (n_i = n_i^0, \forall l' \in [K_n]) \cdot \left[ 1 - 2 \exp \left( -\frac{1}{3} \delta^2 c_1 n \left[ \min_{l' \in [K_n]} q_{l'} \right] \right) \right] \\
\geq \left[ 1 - 2 \exp \left( -\frac{1}{3} \delta^2 (1 - \delta) \rho n \left[ \min_{l' \in [K_n]} \Delta_i \right] \right) \right] \left[ 1 - 2 \exp \left( -\frac{1}{3} \delta^2 c_1 n \left[ \min_{l' \in [K_n]} q_{l'} \right] + \log K_n \right) \right].
\]

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and so by union bound

\[
\Pr \left( (1 - \delta)^2 n \rho \sum_{l' = 1}^{K_n} c_{l} q_{l, l'} \right) \leq N_i \leq (1 + \delta)^2 n \rho \sum_{l' = 1}^{K_n} c_{l} q_{l, l'}, \quad \forall i \in [n] \right)
\]

\[
\geq 1 - 2 \exp \left( -\frac{c_3 \delta^2 (1 - \delta) \rho n \left[ \min_{l \in [K_n]} \Delta_l \right] + \log n \right).
\]

Therefore, with probability approaching one, we have that for \( l \in [K_n] \) and \( i \) such that \( \xi_i \in A_l \) then

\[
\left| N_i \frac{c_1 n \rho}{\sum_{l' = 1}^{K_n} c_{l} q_{l, l'}} \right| \leq (2\delta_n + \delta_n^2) \left[ \sum_{l' = 1}^{K_n} c_{l} q_{l, l'} \right] \leq (2\delta_n + \delta_n^2).
\]

\[
\]

### A.4 Proof of Theorem 1

As in the proof Lemma 2 from Zhang et al. (2015) we obtain the following result.

**Lemma 15.** Assume that \( m \gg n \), then there exists positive constants \( C_1 \) and \( C_2 \) such that with probability at least \( 1 - n^{-C_2} \) the event

\[
\frac{1}{n} \max_{i, j \in [n], i \neq j} \left| \langle A_{i, [m]} , A_{j, [m]} \rangle - \langle \theta_{i, [m]}^*, \theta_{j, [m]}^* \rangle \right| \leq C_1 \left( \frac{\log n}{n} \right)^{\frac{1}{2}}
\]

holds.

As a consequence, we obtain Lemma 2.

**Lemma 16.** Let \( \bar{d}_{i} \) be a distance between \( i, i' \in [n] \backslash [m] \) defined as

\[
\bar{d}_{i}(i, i') = \max_{k \in [m]} \sqrt{\int_0^1 \left[ f_0(\xi_i, t) - f_0(\xi_{i'}, t) \right] f_0(\xi_k, t) dt}.
\]

Then there exist positive constants \( c_1, c_2 > 0 \) such that for large enough \( n \) with probability at least \( 1 - n^{-c_2} \) we have that

\[
\left| \bar{d}_{i}(i, i') - \bar{d}_{i}(i, i') \right| \leq c_1 \left( \frac{\log n}{n} \right)^{1/4} \quad \forall i, i' \in [n] \backslash [m].
\]

**Proof.** We notice that

\[
\left| \bar{d}_{i}(i, i') - \bar{d}_{i}(i, i') \right|^2 \leq \left| \bar{d}_{i}(i, i')^2 - \bar{d}_{i}(i, i')^2 \right|
\]

\[
\leq \max_{k \in [m]} \left| \int_0^1 \left[ f_0(\xi_i, t) - f_0(\xi_{i'}, t) \right] f_0(\xi_k, t) dt \right|
\]

\[
\leq \max_{k \in [m]} \frac{1}{m} \left| \langle \theta_{i, [m]}^*, \theta_{k, [m]}^* \rangle - \langle \theta_{i, [m]}^*, \theta_{k, [m]}^* \rangle \right|
\]

\[
\leq \frac{1}{m} \left| \langle \theta_{i, [m]}^*, \theta_{i, [m]}^* \rangle - \langle \theta_{i, [m]}^*, \theta_{i, [m]}^* \rangle \right|
\]
the claim follows by using Theorem 6 to bound
\[
\left| \int_0^1 [f_0(\xi, t) - f_0(\xi', t)]f_0(\xi_k, t)\, dt - \frac{1}{m} \langle \theta_{i,[m]}^*, \theta_{k,[m]}^* \rangle - \langle \theta_{i',[m]}^*, \theta_{k,[m]}^* \rangle \right|
\]
for any \(i, i' \in [n]\setminus[m], k \in [m]\), which we can do by conditioning on \(\xi, \xi'\) and \(\xi_k\) allowing us to obtain a uniform bound.

\[ \square \]

**Theorem 17.** Let us suppose that Assumptions 1-2 hold. Then, we extend \(\theta^*\) to be in \(\mathbb{R}^{n \times n}\), by setting \(\theta_{i,j}^* = \theta_{i,j}^*\) for all \(i < j\) with \(i, j \in [n]\setminus[m]\). Moreover, we set \(\theta_{i,i}^* = 0\) for all \(i \in [n]\setminus[m]\). Let \(\bar{\tau}\) be constructed as in Section 2.2 by setting \(d := \bar{d}_1\). Then,
\[
\frac{1}{n^2} \sum_{i=1}^{n-m-1} \sum_{j=m+1}^{n} |\theta_{i,j}^* - \theta_{i+1,j}^*| \leq O_P \left( \frac{\log^{(1+\alpha)} n}{n^2} \right).
\]

**Proof.** We first notice that by Theorem 6 we have that with probability approaching one
\[
\max_{i,i' \in [n]\setminus[m]} \left| \frac{1}{n-m} \sum_{j=m+1}^{n} |\theta_{i,j}^* - \theta_{i',j}^*| - \int_0^1 |f_0(\xi', t) - f_0(\xi, t)|\, dt \right| \leq C_1 \left( \frac{\log n}{n} \right)^{1/2}, \tag{26}
\]
for some positive constant \(C_1 > 0\) (we can attain this by first conditioning on \(\xi\)).

On the other hand, with high probability, for any \(i \in [n]\setminus[m]\) we have that by Assumption 1 there exists \(k_i \in [m]\) such that
\[
\left| \int_0^1 (f_0(\xi', t) - f_0(\xi_i, t))f_0(\xi_i, t)\, dt \right| \leq 2\|f_0\|_{\infty} c_1 \left( \frac{\log n}{n} \right)^{\alpha} \tag{27}
\]

Next, for any \(i, i' \in [n]\setminus[m]\) we have that
\[
\int_0^1 |f_0(\xi', t) - f_0(\xi_i, t)|\, dt \leq \left[ \int_0^1 |f_0(\xi', t) - f_0(\xi_i, t)|^2\, dt \right]^{1/2} \\
= \left[ \int_0^1 (f_0(\xi', t) - f_0(\xi_i, t))f_0(\xi_i, t)\, dt + \int_0^1 (f_0(\xi_i, t) - f_0(\xi_i, t))f_0(\xi_i, t)\, dt \right]^{1/2} \\
\leq \left[ \int_0^1 (f_0(\xi', t) - f_0(\xi_i, t))f_0(\xi_i, t)\, dt \right]^{1/2} + \left[ \int_0^1 (f_0(\xi_i, t) - f_0(\xi_i, t))f_0(\xi_i, t)\, dt \right]^{1/2} \\
\leq 2 \left[ \bar{d}_1(i, i')^2 + 2\|f_0\|_{\infty} c_1 \left( \frac{\log n}{n} \right)^{\alpha} \right]^{1/2} \\
\leq 2\bar{d}_1(i, i') + 2\sqrt{2}\|f_0\|_{\infty} c_1 \left( \frac{\log n}{n} \right)^{\alpha/2}. \tag{28}
\]
Therefore, combining (26), (27) and (28) we obtain that with probability approaching 1
\[
\frac{1}{n} \sum_{i=1}^{n-m-1} \sum_{j=m+1}^{n} |\theta^*_{\hat{\tau}(i),j} - \theta^*_{\hat{\tau}(i+1),j}| \leq \sum_{i=1}^{n-m-1} \left[ \int_0^1 |f_0(\xi_{\hat{\tau}(i)},t) - f_0(\xi_{\hat{\tau}(i+1)},t)| dt + C_1 \left( \frac{\log n}{n} \right)^{1/2} \right] \\
\leq \sum_{i=1}^{n-m-1} \left[ 2d_I(\hat{\tau}(i), \hat{\tau}(i+1)) + 2\sqrt{2} \|f_0\|_{\infty} c_1 \left( \frac{\log n}{n} \right)^{\alpha/2} \right] \\
\leq 2 \left( 1 + \frac{\log_2 n}{2} \right) \sum_{i=1}^{n-m-1} d_I(\tau^*(i), \tau^*(i+1)) + C_1 (n \log n)^{1/2} \\
+ 2C_1 n^{3/4} \log^{1/4} n + 2\sqrt{2} \|f_0\|_{\infty} c_1 n^{1-\alpha/2} \log^{\alpha/2} n \\
\leq 2 \left( 1 + \frac{\log_2 n}{2} \right) \max_{k \in [m]} \sqrt{\int_0^1 \left| f_0(\xi_{\tau^*(i)},t) - f_0(\xi_{\tau^*(i+1)},t) \right| dt + \kappa_1 \left( \frac{\log n}{n} \right)^{1/4},
\]
for some positive constant \(\kappa_1\). Therefore, combining with (29)
\[
\frac{1}{n} \sum_{i=1}^{n-m-1} \sum_{j=m+1}^{n} |\theta^*_{\hat{\tau}(i),j} - \theta^*_{\hat{\tau}(i+1),j}| \leq 2 \left( 1 + \frac{\log_2 n}{2} \right) \max_{k \in [m]} \sqrt{\int_0^1 \left| f_0(\xi_{\tau^*(i)},t) - f_0(\xi_{\tau^*(i+1)},t) \right| dt + (2C_1 \kappa_1 + C_1) n^{3/4} \log^{1/4} n + 2\sqrt{2} \|f_0\|_{\infty} c_1 n^{1-\alpha/2} \log^{\alpha/2} n \\
\leq 2 \left( 1 + \frac{\log_2 n}{2} \right) \sqrt{n} \max_{k \in [m]} \left( \sum_{i=1}^{n-m-1} \int_0^1 \left| f_0(\xi_{\tau^*(i)},t) - f_0(\xi_{\tau^*(i+1)},t) \right| dt \right)^{1/2} \\
+ (2C_1 \kappa_1 + C_1) n^{3/4} \log^{1/4} n + 2\sqrt{2} \|f_0\|_{\infty} c_1 n^{1-\alpha/2} \log^{\alpha/2} n
\]
with probability approaching 1. The conclusion follows from Assumption 2.

**Proof of Theorem 1:** This follows combining Theorem 17 with Lemma 8.

**A.5 Proof of Theorem 3**

**Remark 1.** With the notation from Assumption 3, we write \(C_l = \{ i \in [n] : \xi_i \in A_l \} \) and \(n_l = |C_l| \) for \(l \in [K_n] \). Then, we observe that for \(i \in C_l \) and \(i' \in C_{l'} \) the metric \(d_I \) satisfies
\[
d_I(l, l') = d_I(i, i') = \max_{k \in [m]} \left| \sum_{j=1}^{m} \left( \theta^*_{i,j} - \theta^*_{i',j} \right) \theta^*_{k,j} \right| = \max_{k \in [K_n]} \left| \sum_{s=1}^{K_n} \left( Q_{l,s} - Q_{l',s} \right) Q_{k,s} \frac{n_s}{n} \right|
\]
where the second equality holds provided that $C_l \cap [m] \neq \emptyset$ for all $l \in [K_n]$. And so in that case

$$d_I(l, l') \geq \frac{1}{\sqrt{2}} \sqrt{n_s \frac{n_s}{n} (Q_{l,s} - Q_{l',s})^2}.$$  

**Theorem 3**

**Proof.** We use the notation $l(i) \in [K_n]$ if $\xi_i \in A_{l(i)}$. Next, we notice that if $l(i) = l(i')$ we have that $d_I(i, i') = 0$, and so by Lemma 2

$$\hat{d}_I(i, i') \leq \sqrt{2} C_1 \left( \frac{\log n}{n} \right)^{\frac{1}{4}}.$$  

On the other hand if $l(i) \neq l(i')$ we have that

$$\hat{d}_I(i, i') \geq d_I(i, i') - \sqrt{2} C_1 \left( \frac{\log n}{n} \right)^{\frac{1}{4}} > \sqrt{2} C_1 \left( \frac{\log n}{n} \right)^{\frac{1}{4}}$$

with probability approaching 1 which follows from Lemma 2 and Assumption 4. As a result, for large enough $n$, the permutation $\hat{\tau}$ satisfies with probability approaching 1 that there exists $1 \leq i_1 < \ldots < i_{K_n - 1} \leq n - m$ such that

$$\hat{\tau}(s) = \hat{\tau}(s') \text{, } \forall s, s' \leq i_1, \quad \hat{\tau}(s) = \hat{\tau}(s') \text{, } \forall i_r < s \leq s' \leq i_{r+1}, \text{ with } r \in [K_n - 2],$$

and $\hat{\tau}(s) = \hat{\tau}(s') \text{, } \forall s, s' > i_{K_n - 1}$.

Therefore,

$$\frac{1}{n^2} \sum_{i=1}^{n-m} \sum_{j=m+1}^{n} |\theta^*_{\hat{\tau}(i), j} - \theta^*_{\hat{\tau}(i+1), j}| = \frac{1}{n^2} \sum_{j=m+1}^{n} \sum_{l=1}^{K_n-1} |\theta^*_{\hat{\tau}(i), j} - \theta^*_{\hat{\tau}(i+1), j}|$$

$$\leq \frac{1}{n^2} \left[ 2 \, n \, K_n \, \|\theta^*\|_{\infty} \right]$$

$$\leq \frac{2K_n}{n}.$$  

}\end{proof}
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